

```
=> d l1
L1 HAS NO ANSWERS
L1 STR
```

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

```
=> s ll sam sss
MULTIPLE ROLE OQUERIES ARE NOT ALLOWED IN A NON-REACTION FILE
```

```
=> s 11
MULTIPLE ROLE QUERIES ARE NOT ALLOWED IN A NON-REACTION FILE
```

=> file casreact		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	2.30	2.51

FILE 'CASREACT' ENTERED AT 18:40:21 ON 03 AUG 2008  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
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FILE CONTENT:1840 - 3 Aug 2008 VOL 149 ISS 6

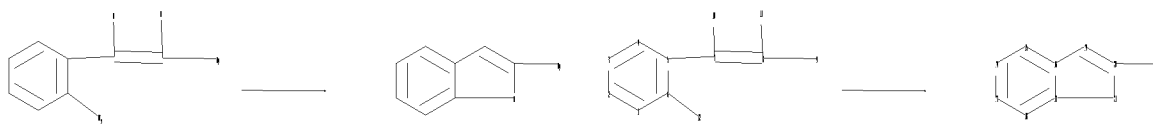
New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*          CASREACT now has more than 15.3 million reactions
*
*****
```

In addition to reactions indexed by CAS, CASREACT contains reactions derived from the following: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=>
Uploading C:\Documents and Settings\EBernhardt\My
Documents\Stnexp\Queries\10557537-II.str
```



```

chain nodes :
7 8 9 10 11 12 22
ring nodes :
1 2 3 4 5 6 13 14 15 16 17 18 19 20 21
chain bonds :
5-7 6-12 7-8 7-10 8-9 8-11 20-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 16-19 17-18
17-21 19-20 20-21
exact/norm bonds :
8-9 16-19 17-21 19-20 20-21 20-22
exact bonds :
5-7 6-12 7-8 7-10 8-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

```

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom
Generic attributes :
9:
Saturation          : Unsaturated
22:
Saturation          : Unsaturated

```

```

fragments assigned product role:
containing 13
fragments assigned reactant/reagent role:
containing 1

```

L2 STRUCTURE UPLOADED

=> s 12

SAMPLE SEARCH INITIATED 18:40:57 FILE 'CASREACT'  
 SCREENING COMPLETE - 493 REACTIONS TO VERIFY FROM 56 DOCUMENTS

100.0% DONE 493 VERIFIED 0 HIT RXNS 0 DOCS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED VERIFICATIONS: 8529 TO 11191  
 PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L2 ( 0 REACTIONS)

=> s l2 sss full

FULL SEARCH INITIATED 18:41:06 FILE 'CASREACT'

SCREENING COMPLETE - 13464 REACTIONS TO VERIFY FROM 1374 DOCUMENTS

100.0% DONE 13464 VERIFIED 88 HIT RXNS

18 DOCS

SEARCH TIME: 00.00.05

L4 18 SEA SSS FUL L2 ( 88 REACTIONS)

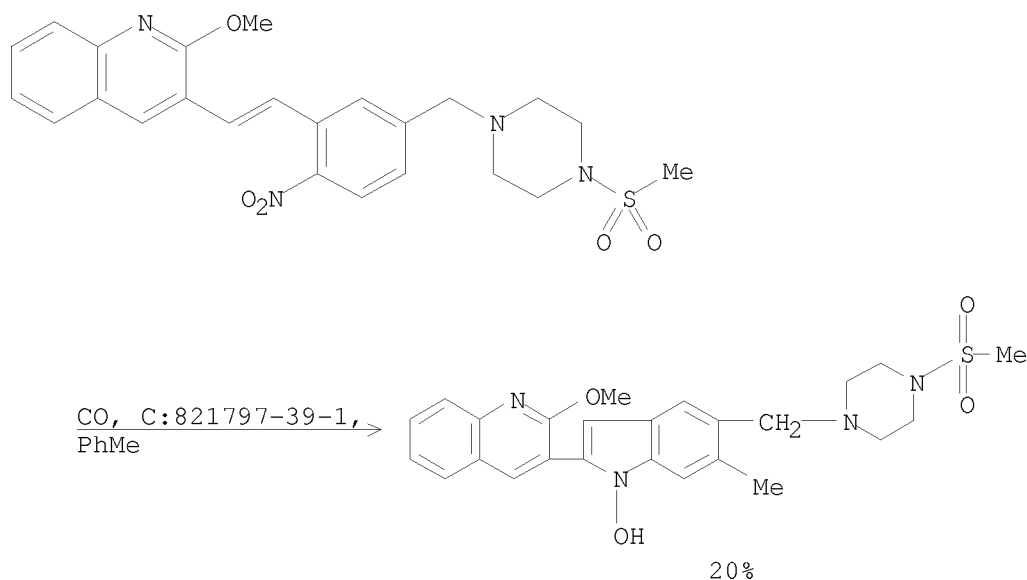
=> d scan 1-18

'1-18' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

II Substituted indoles and a process for their preparation via  
Pd/diamine-catalyzed reductive cyclization of ortho-nitrostyrenes under CO  
pressure

RX(5) OF 30



NOTE: Endeavor reactor was used

The following are valid formats:

ABS ----- GI and AB  
ALL ----- BIB, AB, IND, RE, Single-step Reactions  
APPS ----- AI, PRAI  
BIB ----- AN, plus Bibliographic Data  
CAN ----- List of CA abstract numbers without answer numbers  
CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels

IBIB ----- BIB, indented with text labels  
 IND ----- Indexing data  
 IPC ----- International Patent Classifications  
 ISTD ----- STD, indented with text labels  
 OBIB ----- AN, plus Bibliographic Data (original)  
 OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations  
 SIBIB ----- IBIB, no citations

MAX ----- Same as ALL  
 PATS ----- PI, SO  
 SCAN ----- TI and FCRD (random display, no answer number. SCAN  
                   must be entered on the same line as DISPLAY, e.g.,  
                   D SCAN.)  
 SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for  
                   all single-step reactions)  
 STD ----- BIB, IPC, and NCL

CRD ----- Compact Display of All Hit Reactions  
 CRDREF ----- Compact Reaction Display and SO, PY for Reference  
 FHIT ----- Reaction Map, Diagram, and Summary for first  
                   hit reaction  
 FHITCBIB --- FHIT, AN plus CBIB  
 FCRD ----- First hit in Compact Reaction Display (CRD) format  
 FCRDREF ----- First hit in Compact Reaction Display (CRD) format with  
                   CA reference information (SO, PY). (Default)  
 FPATH ----- PATH, plus Reaction Summary for the "long path"  
 FSPATH ----- SPATH, plus Reaction Summary for the "short path"  
 HIT ----- Reaction Map, Reaction Diagram, and Reaction  
                   Summary for all hit reactions and fields containing  
                   hit terms  
 OCC ----- All hit fields and the number of occurrences of the  
                   hit terms in each field. Includes total number of  
                   HIT, PATH, SPATH reactions. Labels reactions that have  
                   incomplete verifications.  
 PATH ----- Reaction Map and Reaction Diagram for the "long  
                   path". Displays all hit reactions, except those  
                   whose steps are totally included within another hit  
                   reaction which is displayed  
 RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)  
 RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
 RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
 RXS ----- Hit Reaction Summaries (Map and Summary for all hit reactions)  
 SPATH ----- Reaction Map and Reaction Diagram for the "short  
                   path". Displays all single step reactions which  
                   contain a hit substance. Also displays those  
                   multistep reactions that have a hit substance in both  
                   the first and last steps of the reaction, except for  
                   those hit reactions whose steps are totally included  
                   within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH,

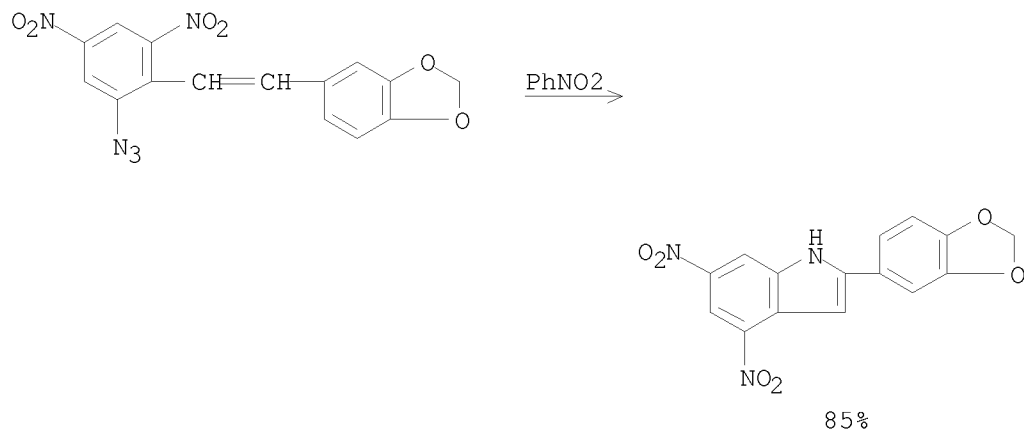
FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):17

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis of 2-aryl- and 2-hetaryl-4,6-dinitroindoles from 2,4,6-trinitrotoluene

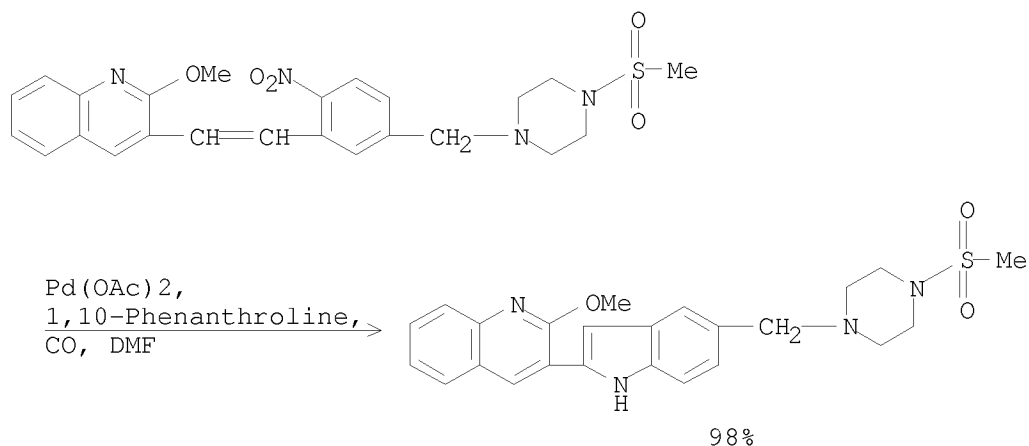
RX(22) OF 57



L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI A highly active catalyst for the reductive cyclization of ortho-nitrostyrenes under mild conditions

RX(1) OF 47

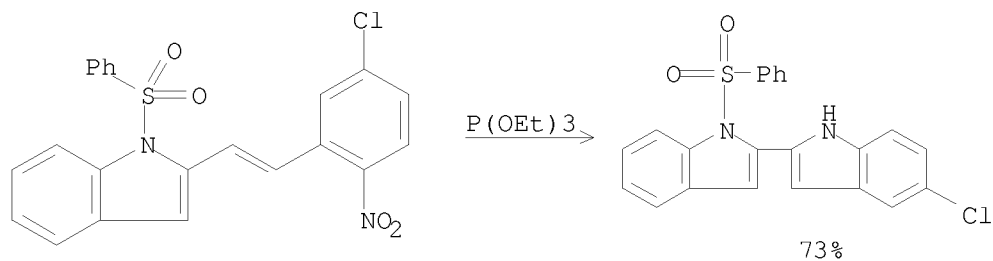


NOTE: optimization study, green chem. - waste reduction

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Effective Strategy for the Preparation of Indolocarbazole Aglycons and Glycosides: Total Synthesis of Tjipanazoles B, D, E, and I

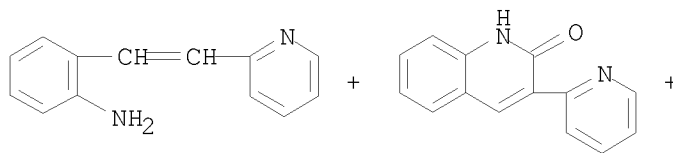
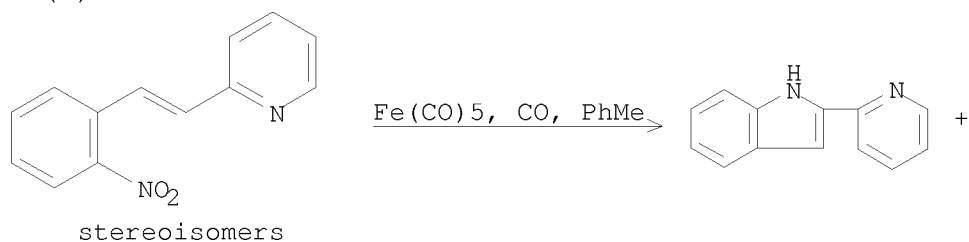
RX(3) OF 71



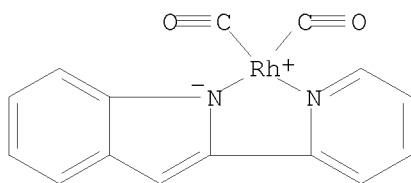
L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Deoxygenation reactions of ortho-nitrostyrenes with carbon monoxide catalyzed by metal carbonyls: a new route to indoles

RX(8) OF 12



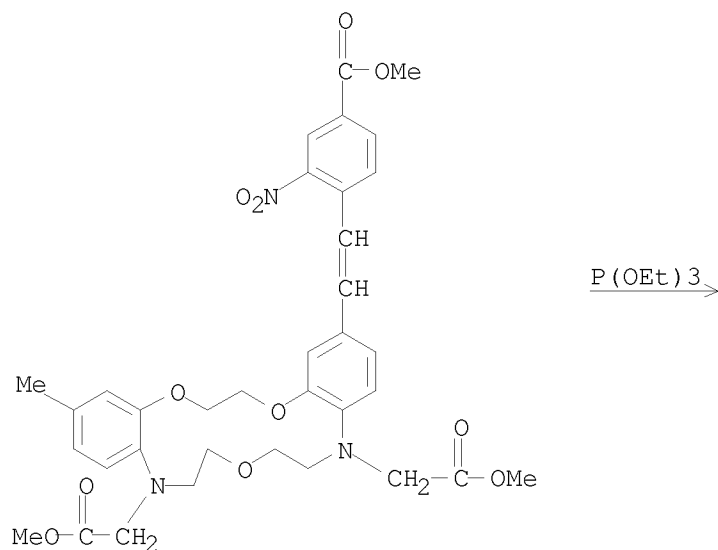
RX(8) OF 12



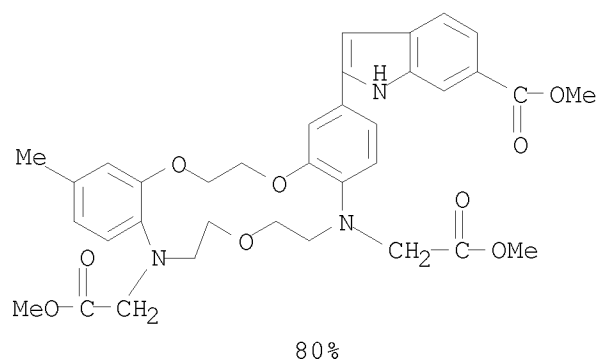
L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Preparation of crown ether derivatives as metal chelating agents

RX(26) OF 555



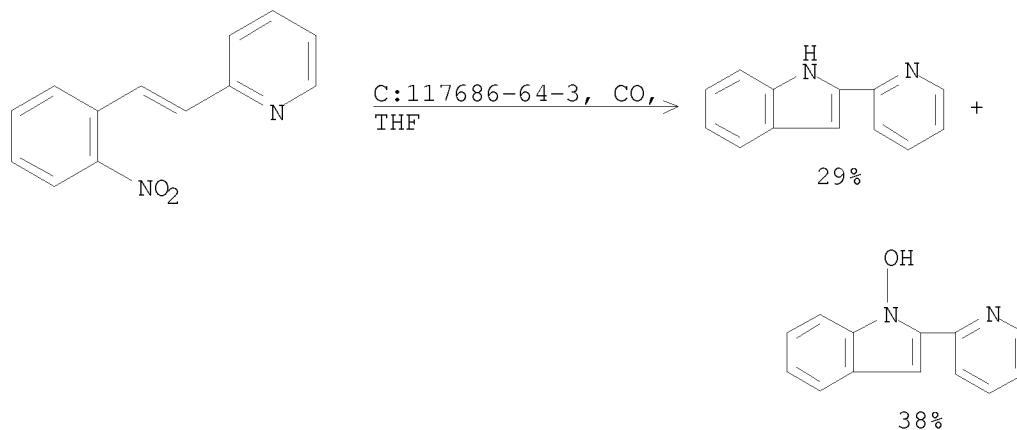
RX(26) OF 555



L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI The unprecedented detection of the intermediate formation of N-hydroxy derivatives during the carbonylation of 2'-nitrochalcones and 2-nitrostyrenes catalyzed by palladium

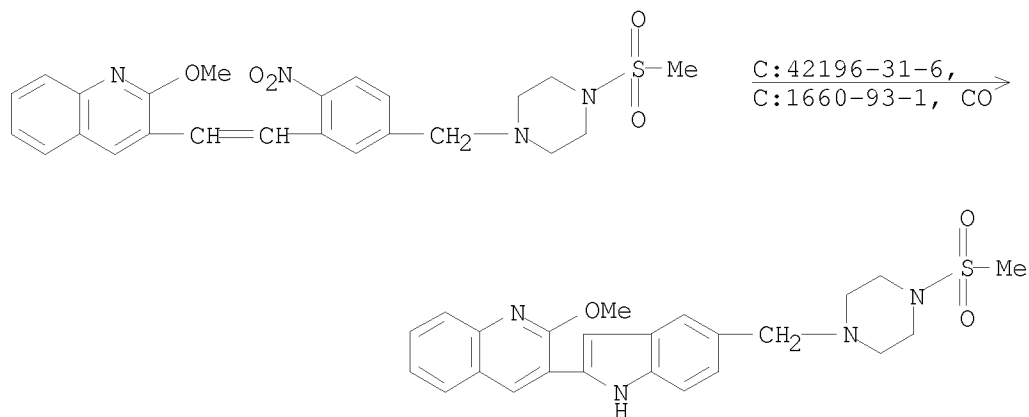
RX(4) OF 5



L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Applying statistical design of experiments and automation to the rapid optimization of metal-catalyzed processes in process development

RX(2) OF 2



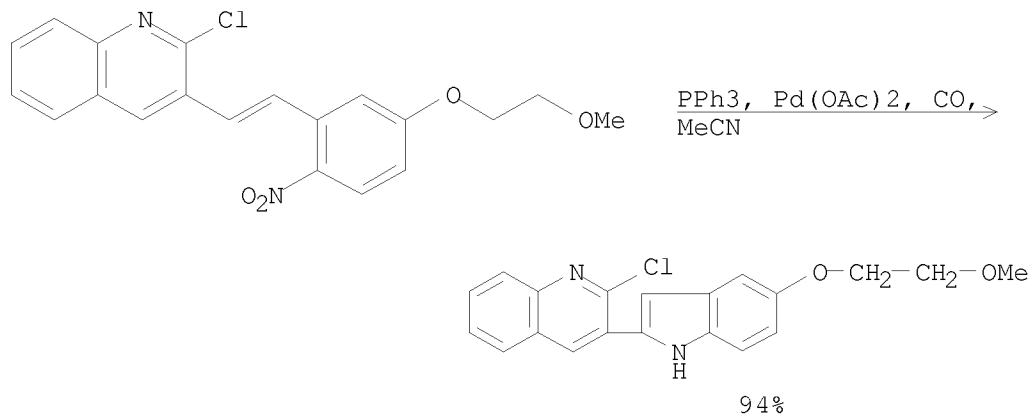
NOTE: optimization study, optimized on catalyst loading, optimized on pressure, optimized on temperature

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Rapid and Efficient Synthesis of 1H-Indol-2-yl-1H-quinolin-2-ones



RX(4) OF 63

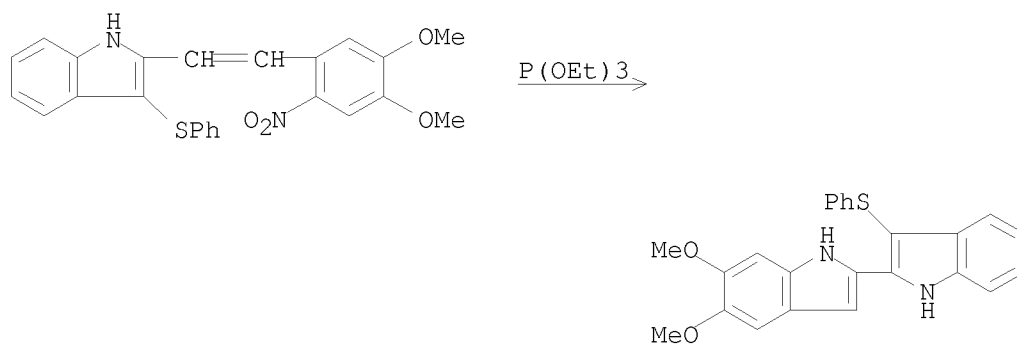


NOTE: alternative prepn. shown

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis of 2,2'-biindolyis; potential intermediates for indolocarbazole alkaloids

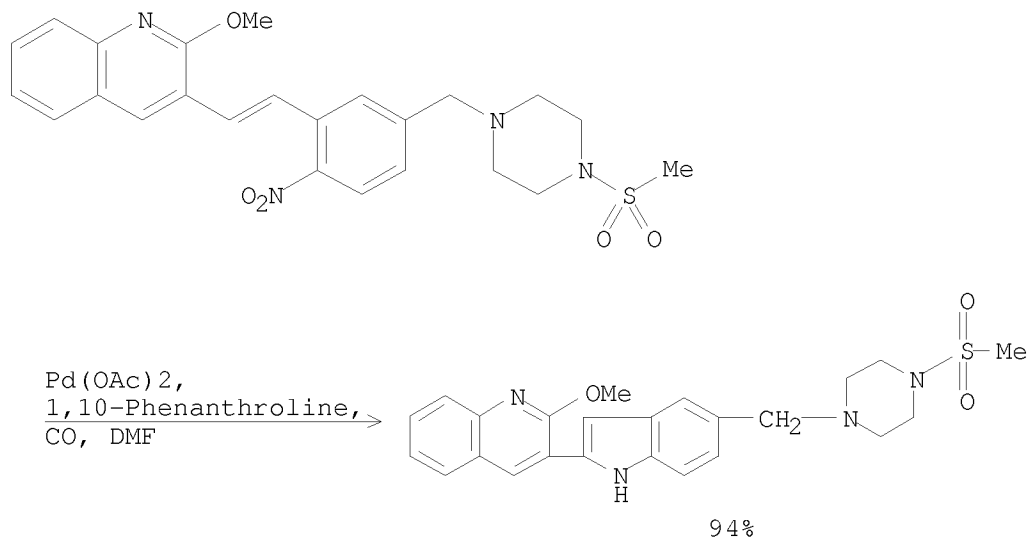
RX(2) OF 6



L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis of 5-Substituted-1H-indol-2-yl-1H-quinolin-2-ones: A Novel Class of KDR Kinase Inhibitors

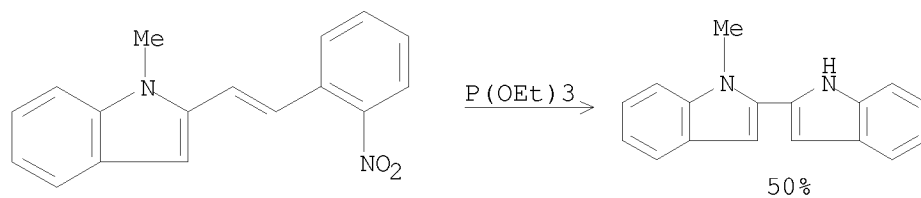
RX(36) OF 350



L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Benzannulation reactions of Fischer carbene complexes for the synthesis of indolocarbazoles

RX(10) OF 177

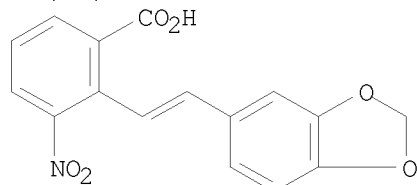


NOTE: thermal, alternative preps. gave similar yields

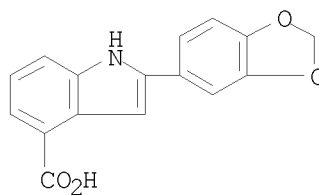
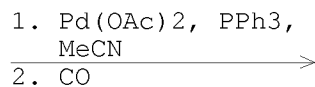
L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Preparation of 2-arylindole-4-carboxylic amide derivatives

RX(15) OF 47



(step 1)

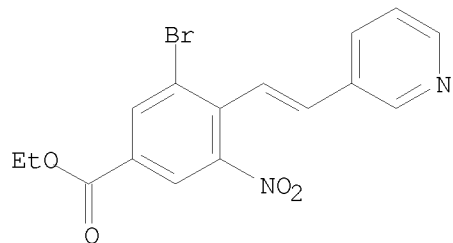


92%

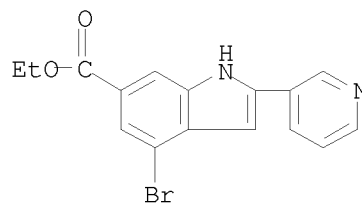
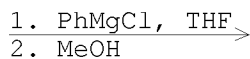
L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Mild synthesis of polyfunctional benzimidazoles and indoles by the reduction of functionalized nitroarenes with phenylmagnesium chloride

RX(37) OF 85



(step 1)

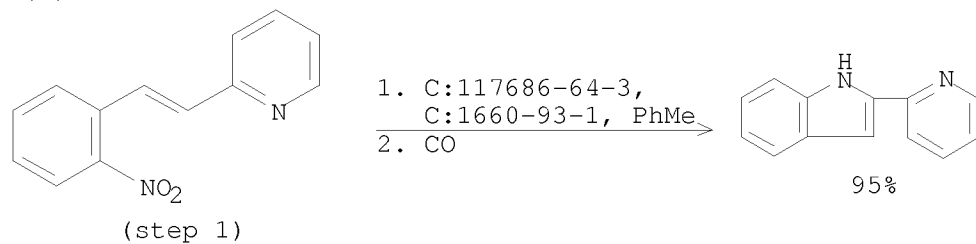


70%

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis of 2-heteroaryl-substituted indoles via palladium-catalyzed reductive N-heterocyclization

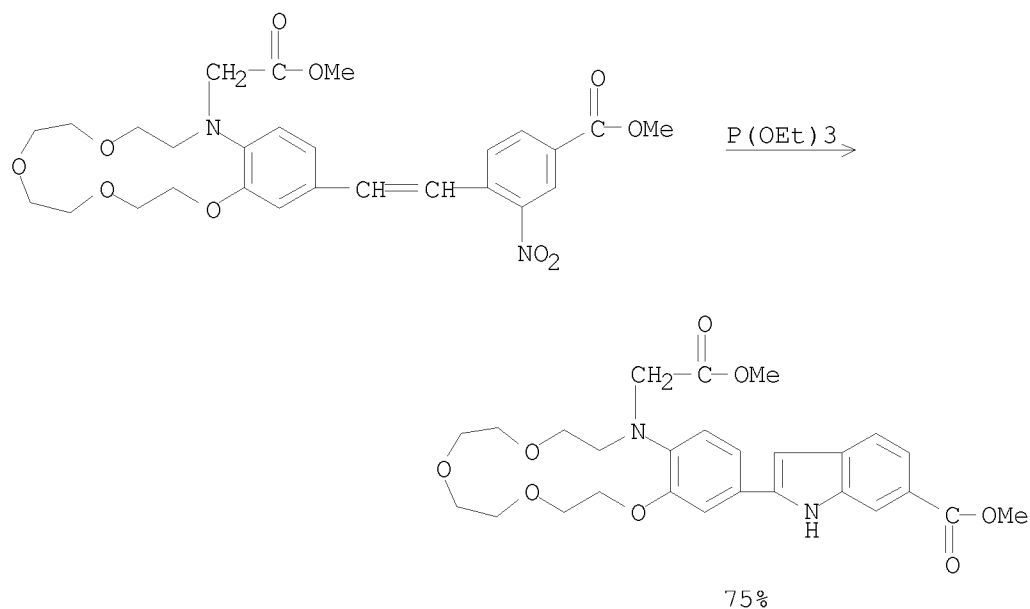
RX(1) OF 9



L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Fluorescent metal ion indicators based on benzoannelated crown systems: a green fluorescent indicator for intracellular sodium ions

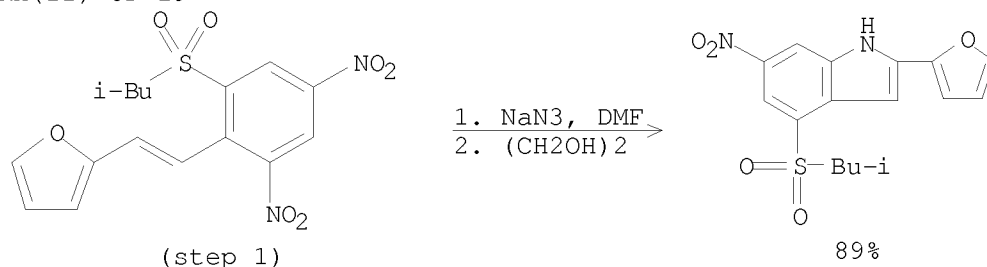
RX(28) OF 161



L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Interaction of 2,4,6-trinitrotoluene and its analogs with aldehydes. Synthesis of benzo-annelated heterocycles from the products of condensation

RX(11) OF 29

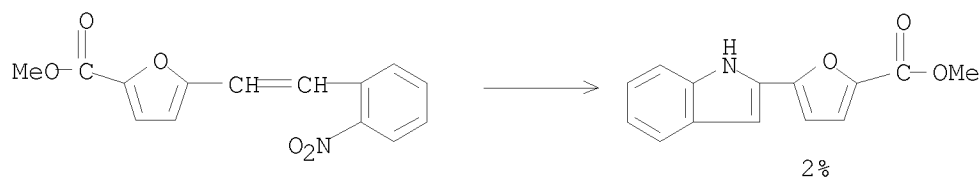


NOTE: regioselective, thermal, stereoselective

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Intramolecular ring formation of phenyl azide and furan moieties

RX(69) OF 98 - 3 STEPS

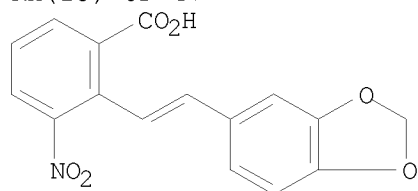


ALL ANSWERS HAVE BEEN SCANNED

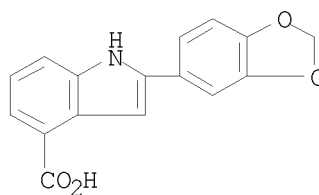
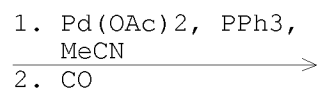
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L4 ANSWER 1 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(15) OF 47



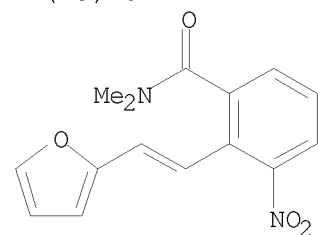
(step 1)



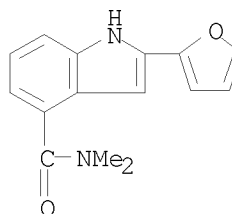
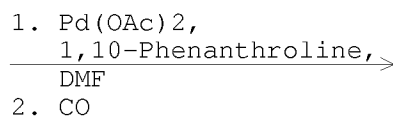
92%

CON: STAGE(1) room temperature -> 70 deg C  
STAGE(2) 16 hours, 70 deg C, 60 psi

RX(23) OF 47



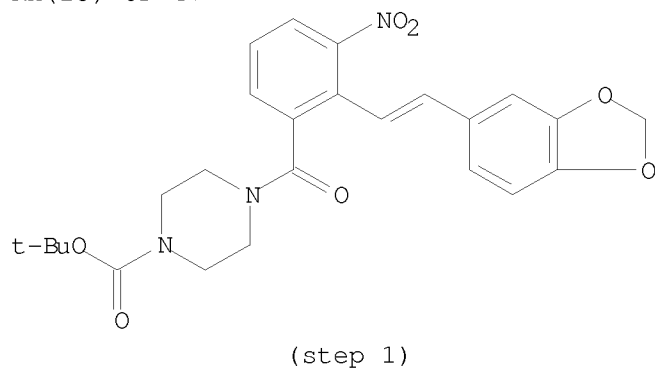
(step 1)



98%

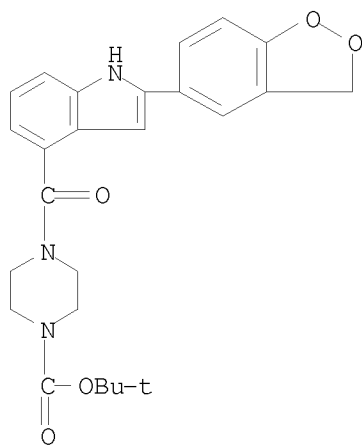
CON: STAGE(1) room temperature -> 80 deg C  
STAGE(2) 16 hours, 80 deg C, 30 psi

RX(25) OF 47



1. Pd(OAc)<sub>2</sub>,  
1,10-Phenanthroline,  
DMF  
2. CO

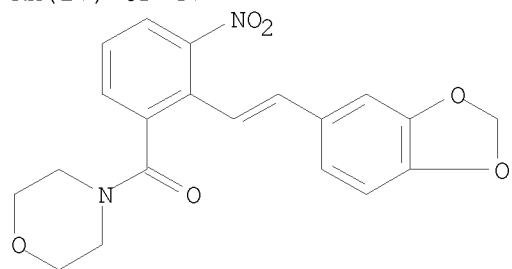
RX(25) OF 47



99%

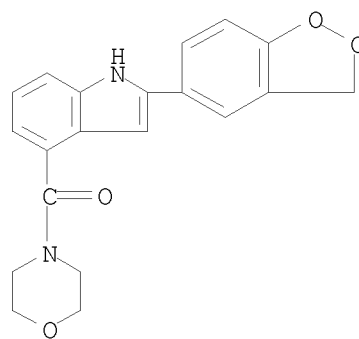
CON: STAGE(1) room temperature -> 80 deg C  
STAGE(2) 16 hours, 80 deg C, 30 psi

RX(27) OF 47



(step 1)

1. Pd(OAc)<sub>2</sub>,  
1,10-Phenanthroline,  
DMF  
2. CO

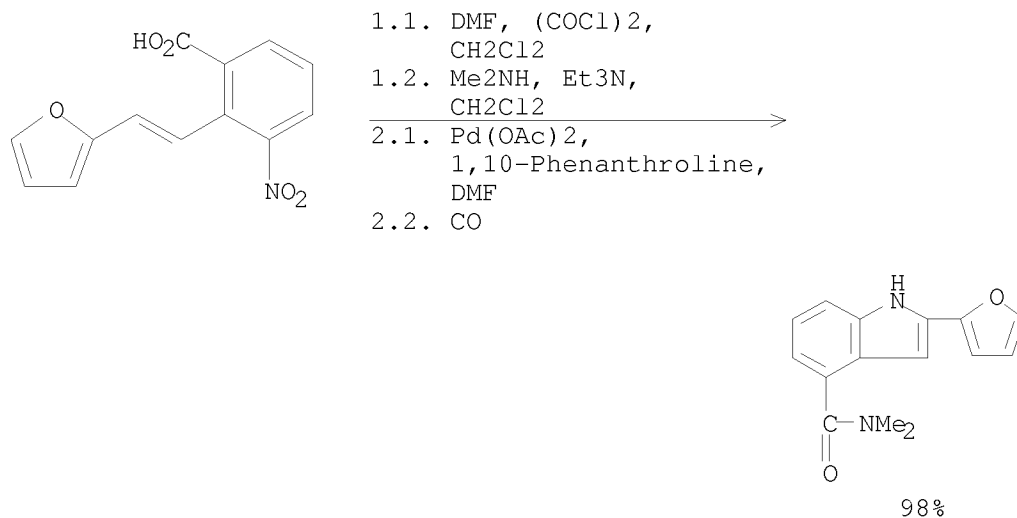


98%

CON: STAGE(1) room temperature -> 80 deg C  
STAGE(2) 16 hours, 80 deg C, 30 psi

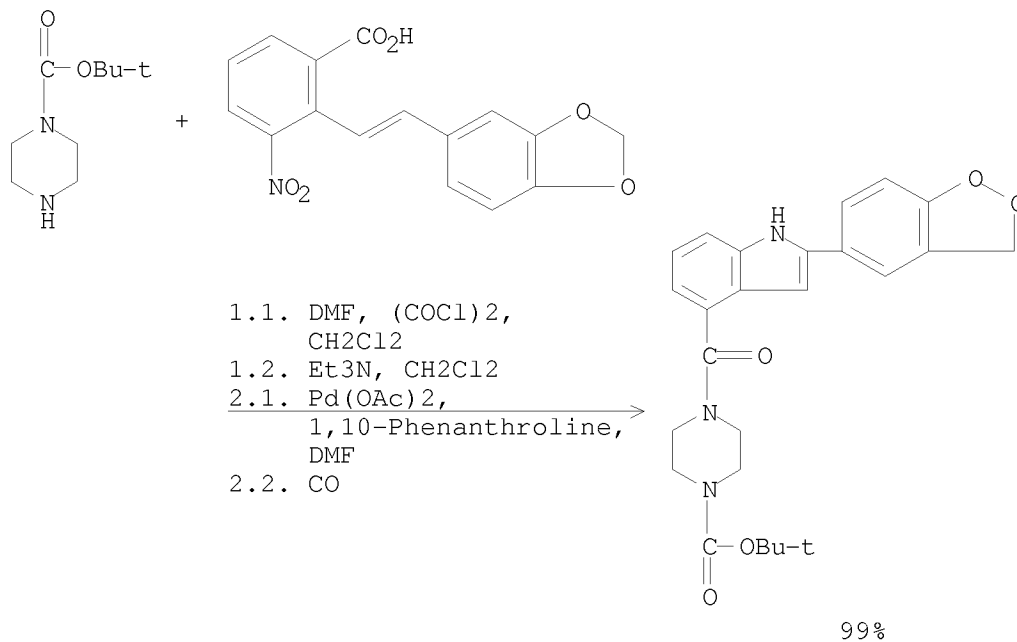


RX(37) OF 47 - 2 STEPS



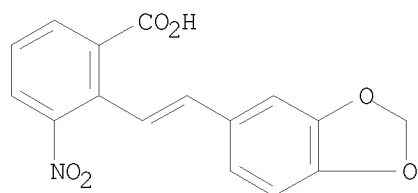
CON: STEP(1.1) 1.5 hours, room temperature  
 STEP(1.2) room temperature; 30 minutes, room temperature  
 STEP(2.1) room temperature -> 80 deg C  
 STEP(2.2) 16 hours, 80 deg C, 30 psi

RX(39) OF 47 - 2 STEPS

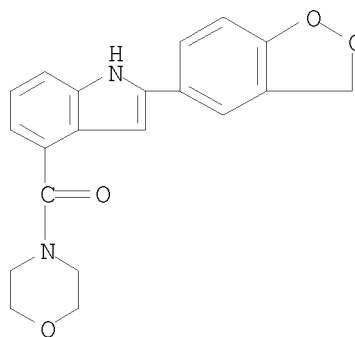


CON: STEP(1.1) 1.5 hours, room temperature  
STEP(1.2) room temperature; 30 minutes, room temperature  
STEP(2.1) room temperature -> 80 deg C  
STEP(2.2) 16 hours, 80 deg C, 30 psi

RX(41) OF 47 - 2 STEPS



1.1. DMF, (COCl)<sub>2</sub>,  
CH<sub>2</sub>Cl<sub>2</sub>  
1.2. Morpholine, Et<sub>3</sub>N,  
CH<sub>2</sub>Cl<sub>2</sub>  
2.1. Pd(OAc)<sub>2</sub>,  
1,10-Phenanthroline,  
DMF  
2.2. CO



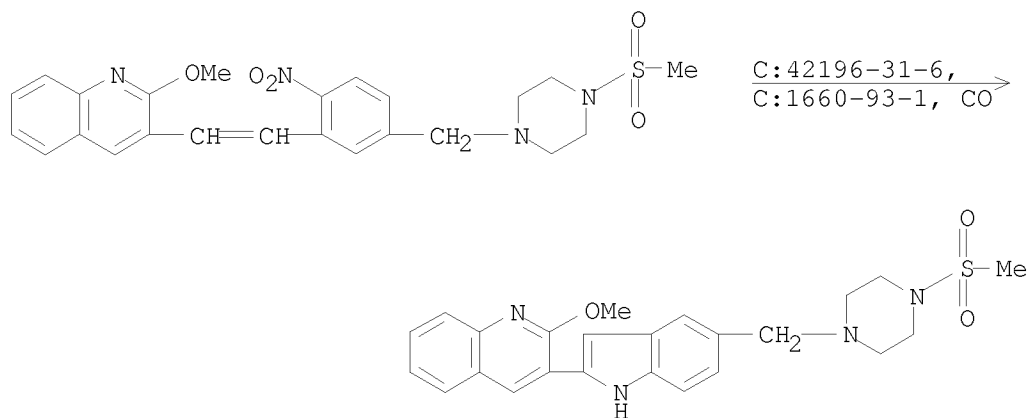
98%

CON: STEP(1.1) 1.5 hours, room temperature  
STEP(1.2) room temperature; 30 minutes, room temperature  
STEP(2.1) room temperature -> 80 deg C  
STEP(2.2) 16 hours, 80 deg C, 30 psi

=> d crd 2-18

L4 ANSWER 2 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

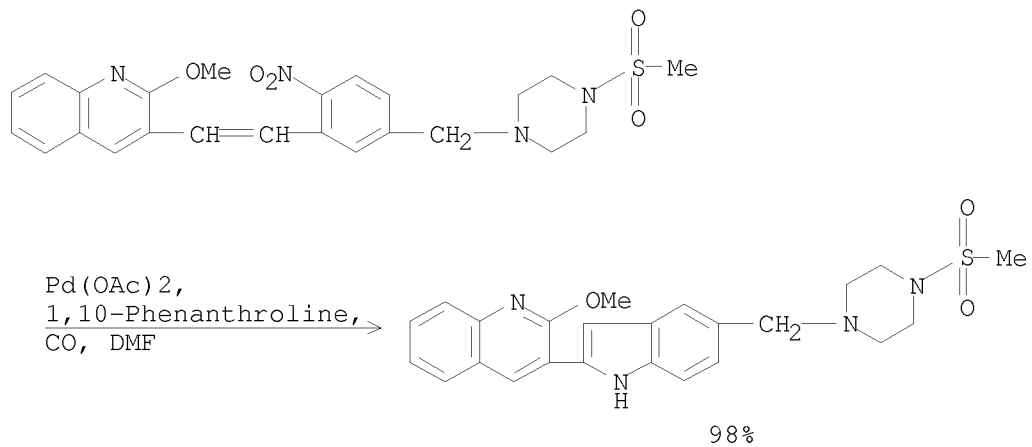
RX (2) OF 2



NOTE: optimization study, optimized on catalyst loading, optimized on  
pressure, optimized on temperature  
CON: 70 - 80 deg C, 15 psi

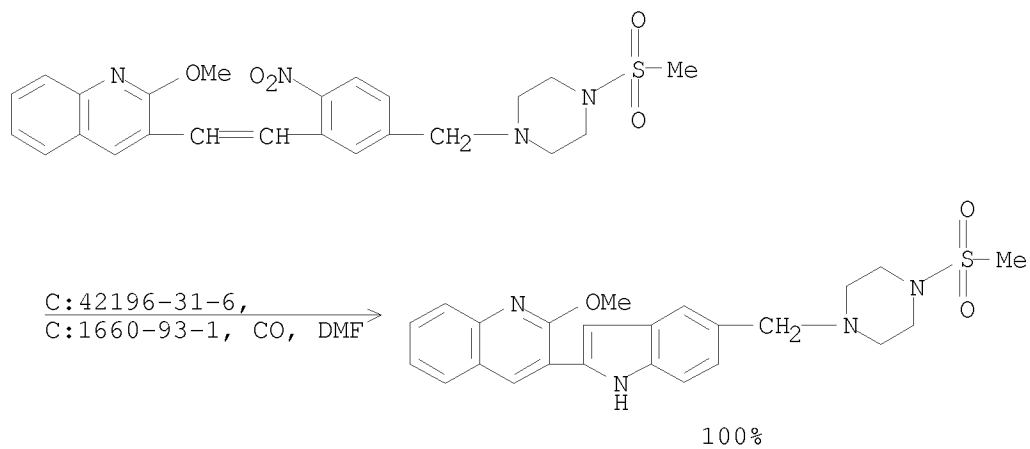
L4 ANSWER 3 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX (1) OF 47



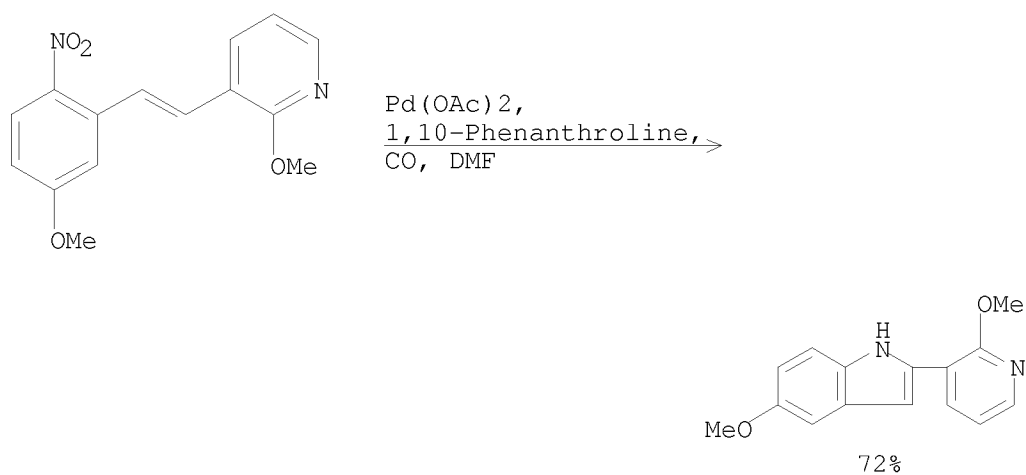
NOTE: optimization study, green chem. - waste reduction  
CON: 70 deg C, 15 psi

RX(2) OF 47



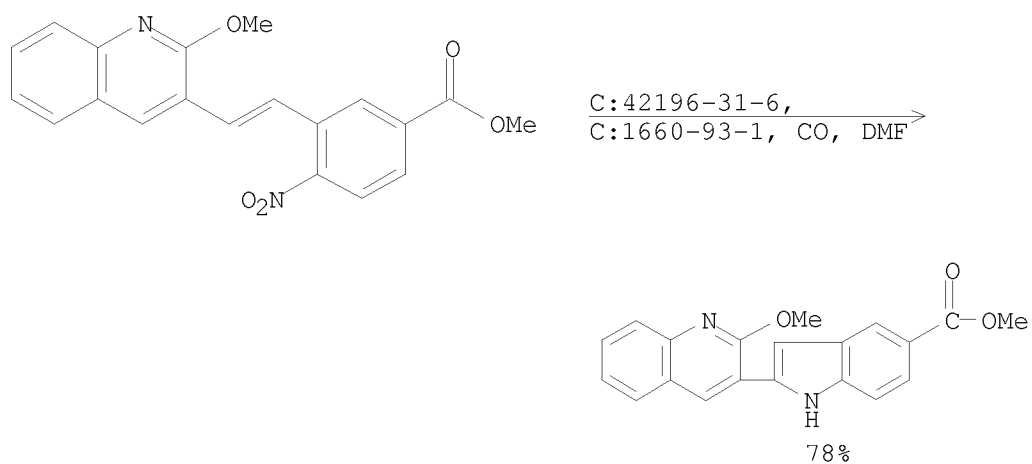
NOTE: optimization study, green chem. - waste reduction  
 CON: 70 deg C, 15 psi

RX(23) OF 47



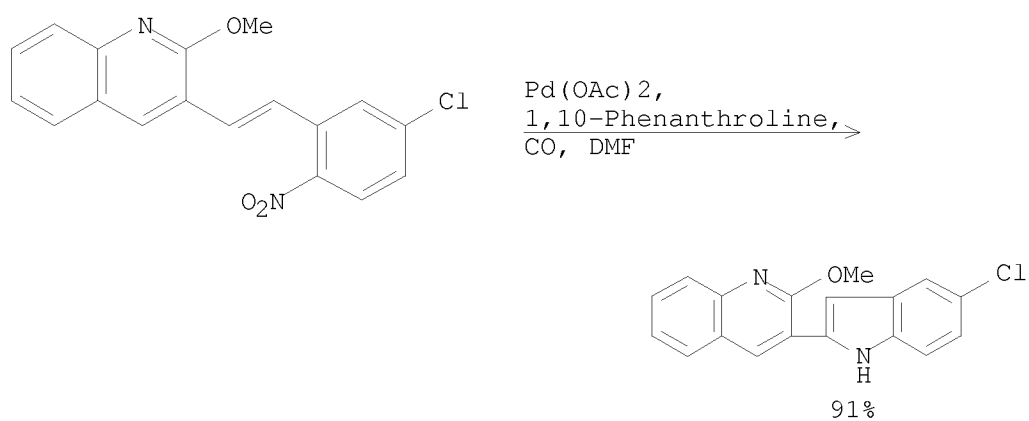
NOTE: green chem. - waste reduction  
 CON: 16 hours, 70 deg C, 30 psi

RX(24) OF 47



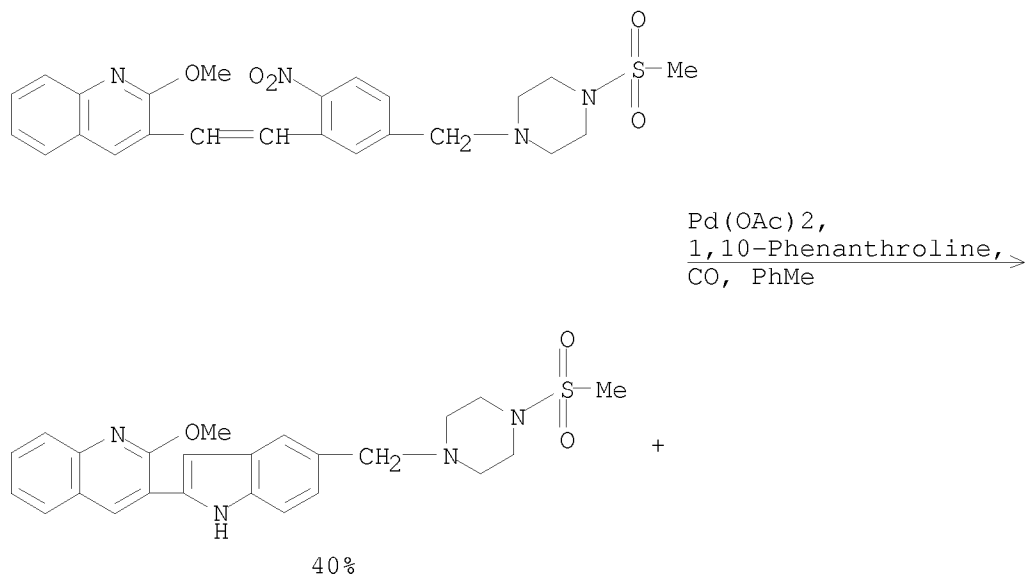
NOTE: green chem. - waste reduction  
 CON: 16 hours, 80 deg C, 15 psi

RX(25) OF 47

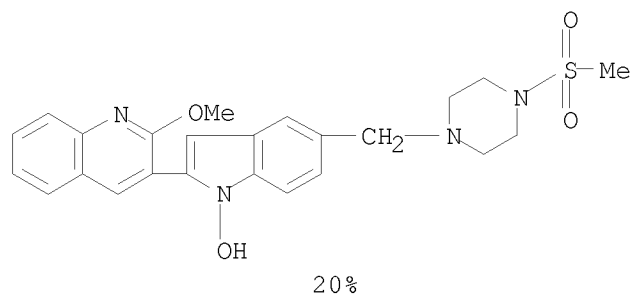


NOTE: green chem. - waste reduction  
 CON: 16 hours, 80 deg C, 15 psi

RX(28) OF 47

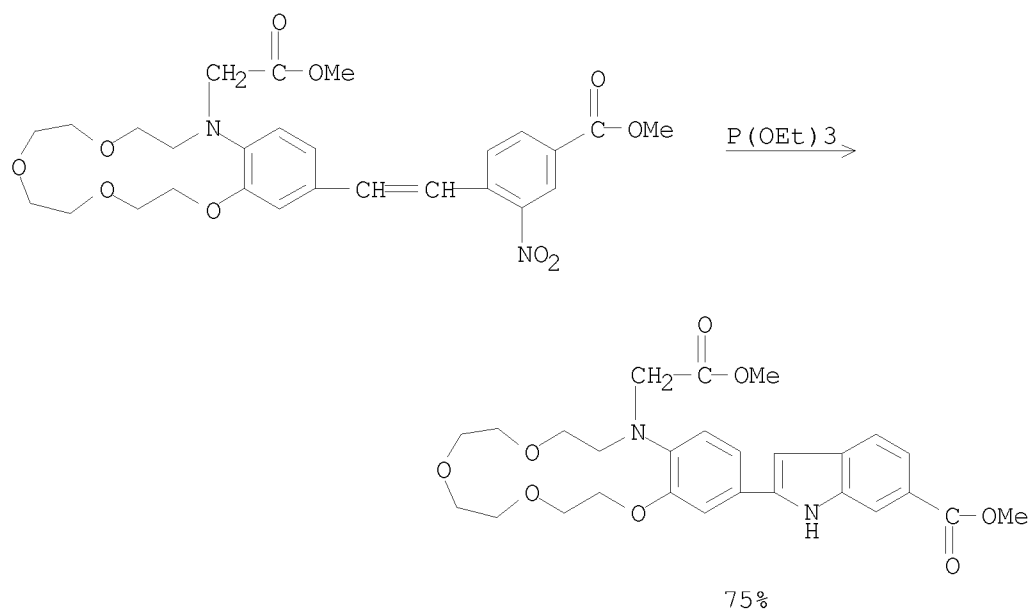


RX(28) OF 47

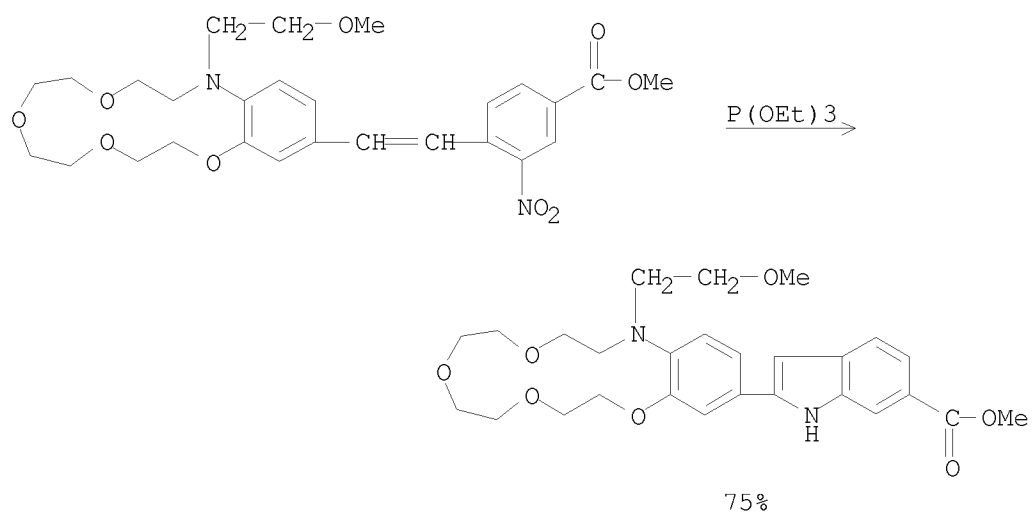


CON: 70 deg C, 15 psi

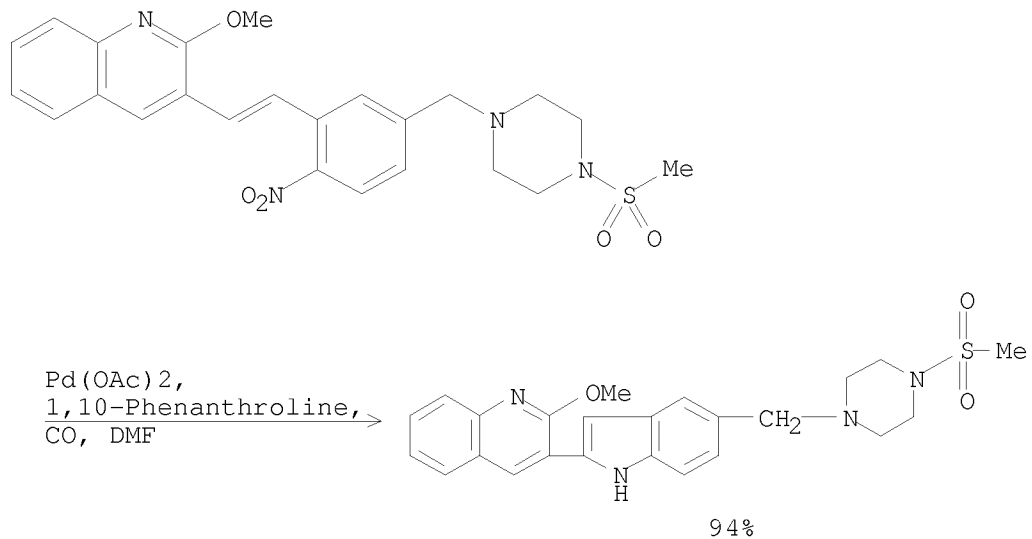
RX(28) OF 161



RX(29) OF 161

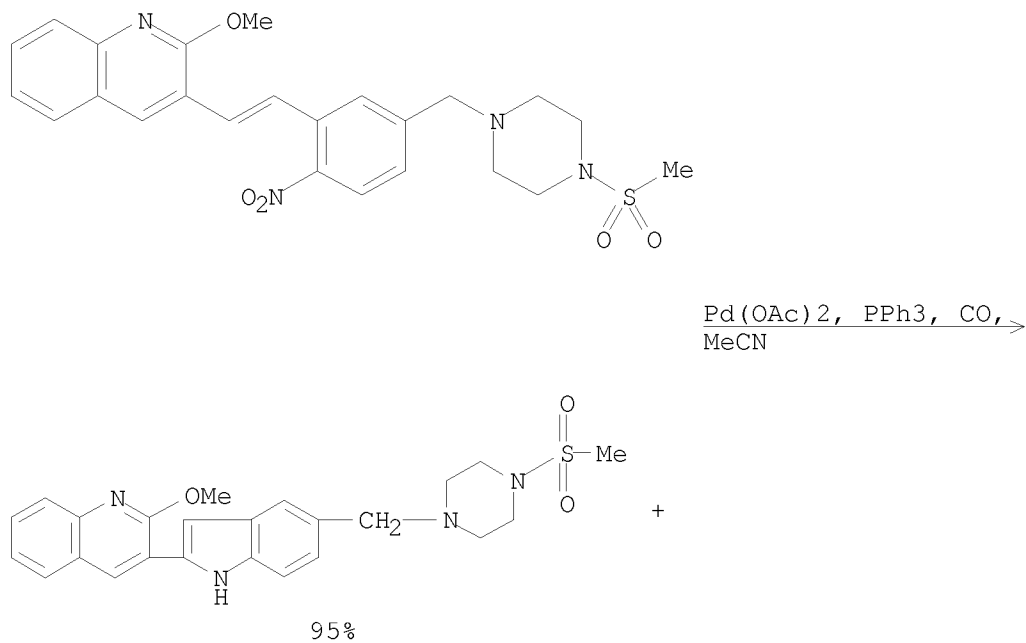


RX(36) OF 350



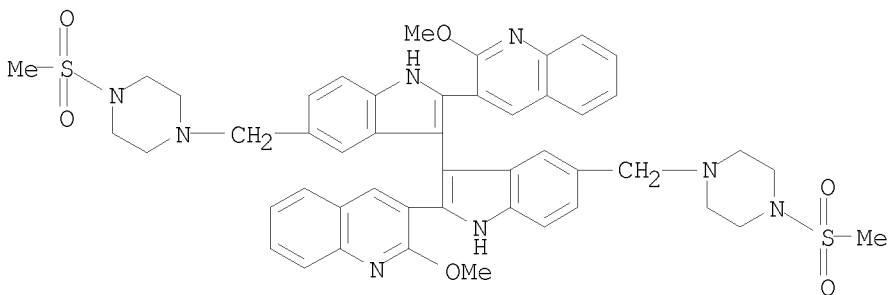
CON: 14 hours, 70 deg C, 15 psi

RX(37) OF 350



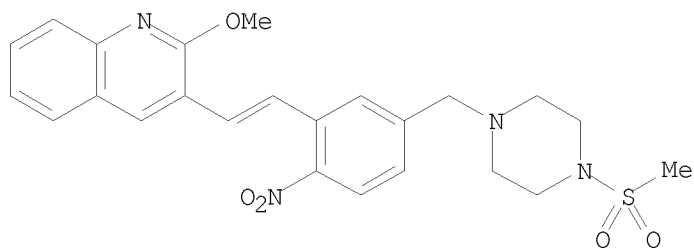


RX(37) OF 350



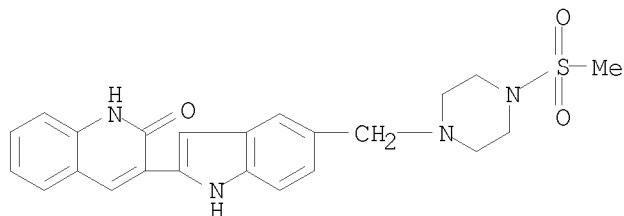
CON: 15 hours, 70 deg C, 60 atm

RX(59) OF 350 - 2 STEPS



1. Pd(OAc)<sub>2</sub>,  
1,10-Phenanthroline,  
CO, DMF  
2. HCl, Water, DMF

RX(59) OF 350 - 2 STEPS

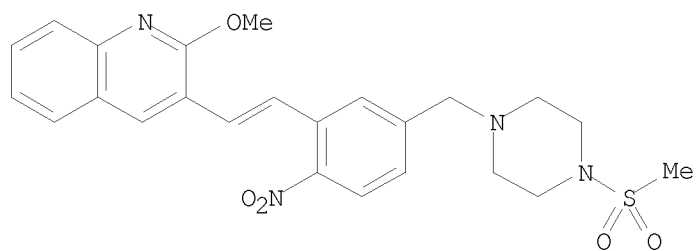


HCl  
100%

CON: STEP(1) 14 hours, 70 deg C, 15 psi

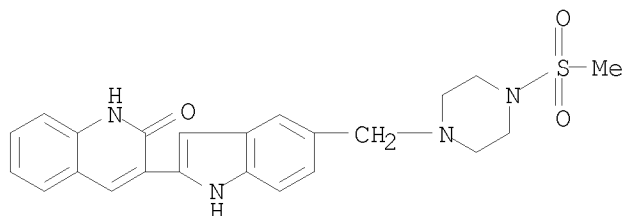
10/557537- Part II

RX(60) OF 350 - 2 STEPS



1. Pd(OAc)<sub>2</sub>, PPh<sub>3</sub>, CO,  
MeCN  
2. HCl, Water, DMF →

RX(60) OF 350 - 2 STEPS

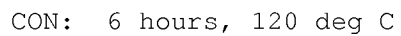
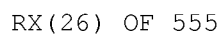


HCl

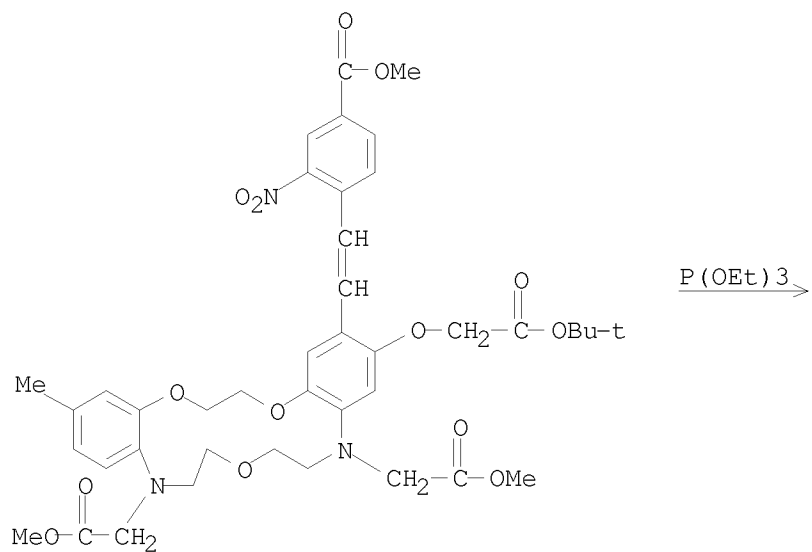
100%

CON: STEP(1) 15 hours, 70 deg C, 60 atm

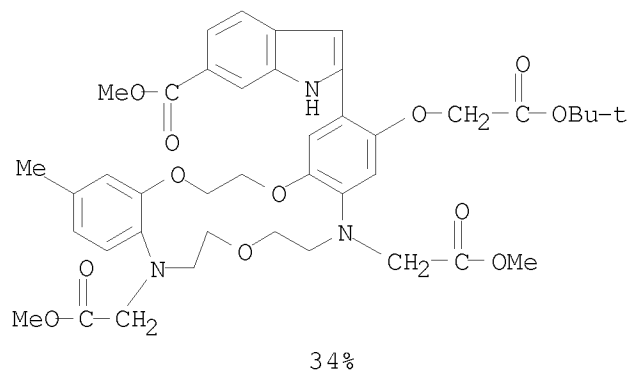
L4 ANSWER 6 OF 18 CASREACT COPYRIGHT 2008 ACS on STN



RX(48) OF 555



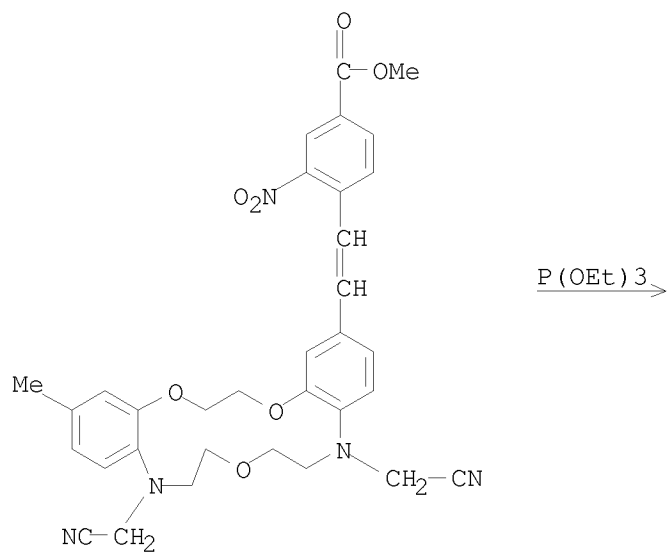
RX(48) OF 555



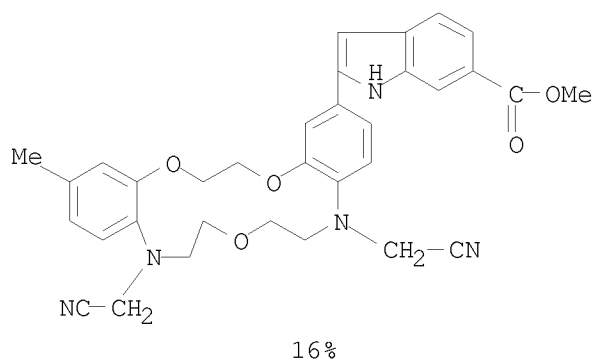
34%

CON: 7 hours, 130 deg C

RX(54) OF 555

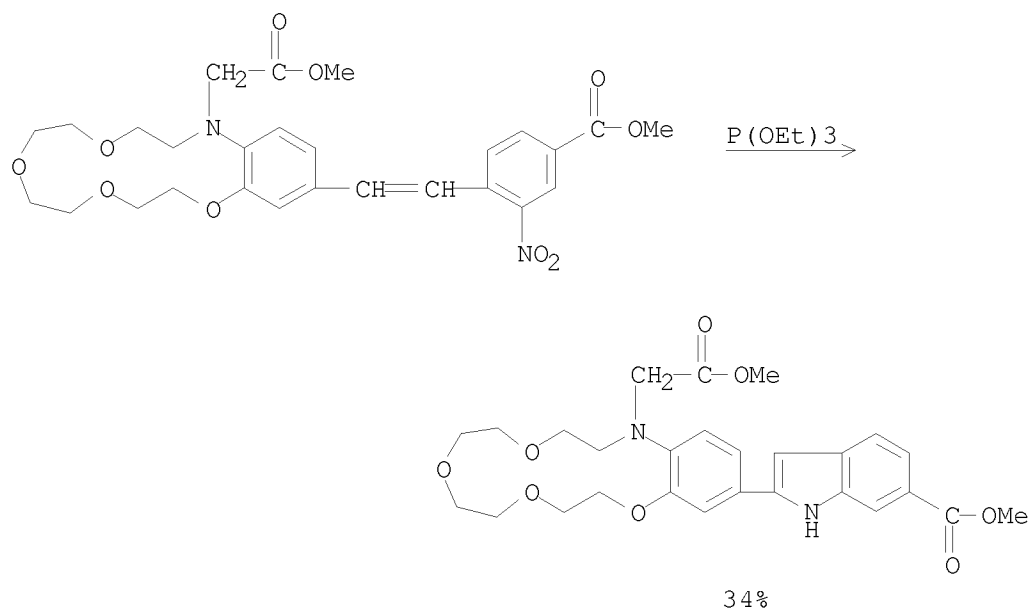


RX(54) OF 555



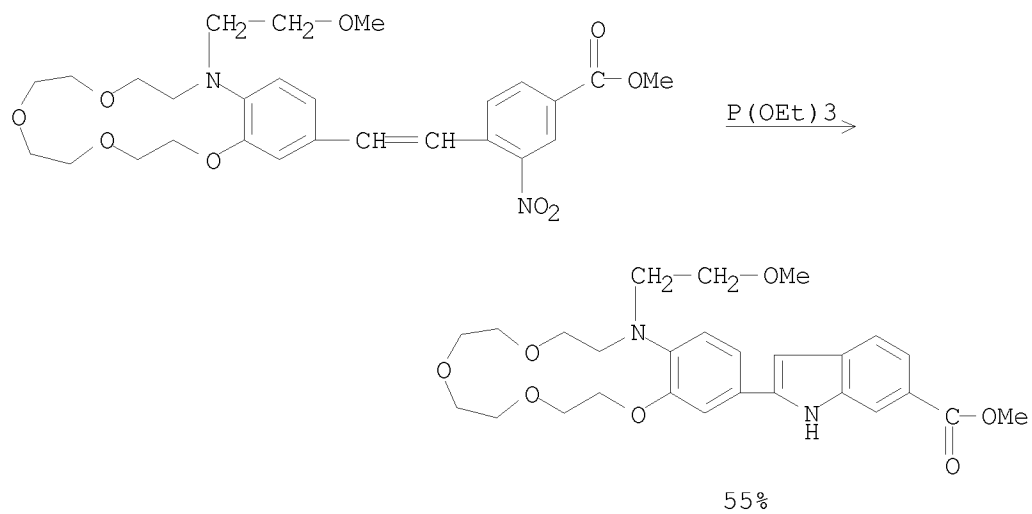
CON: 16 hours, 120 deg C

RX(67) OF 555



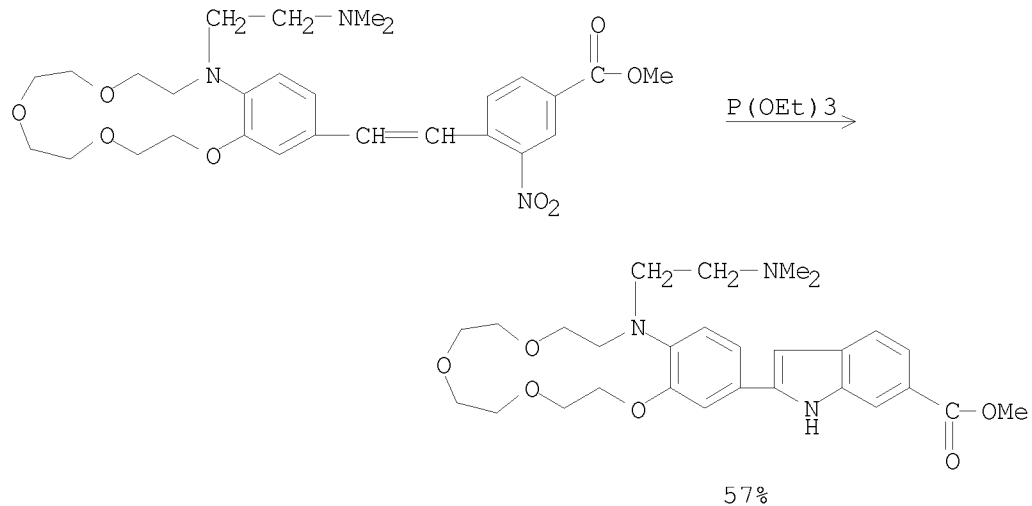
CON: 4 hours, 125 deg C

RX(91) OF 555



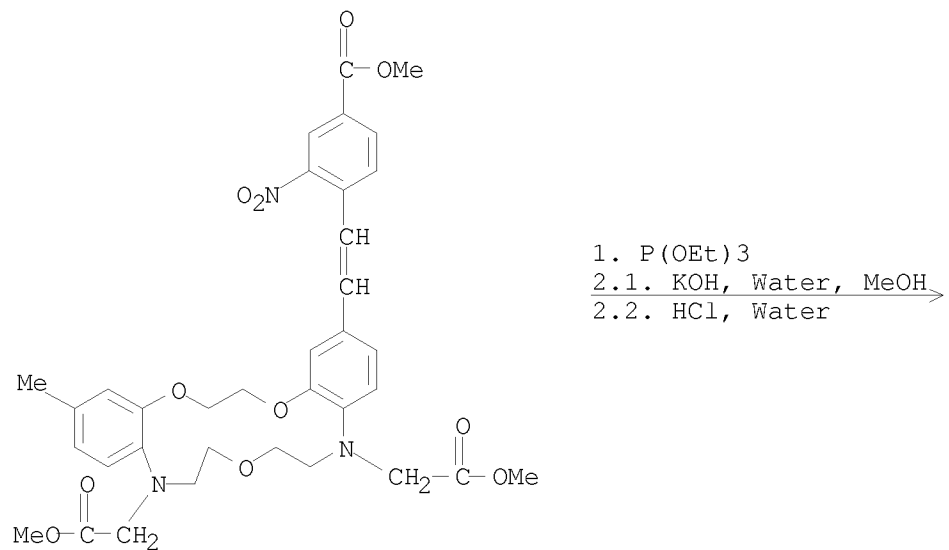
CON: 4 hours, 125 deg C

RX (97) OF 555

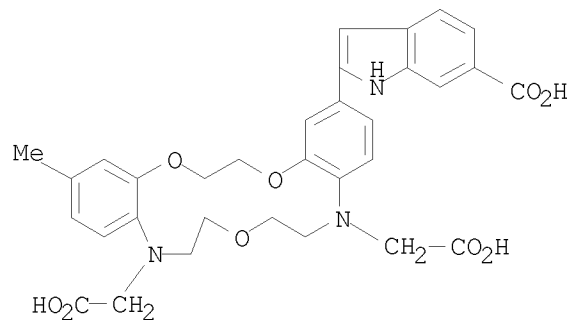


CON: 14 hours, 125 deg C

RX(132) OF 555 - 2 STEPS



## RX(132) OF 555 - 2 STEPS



57%

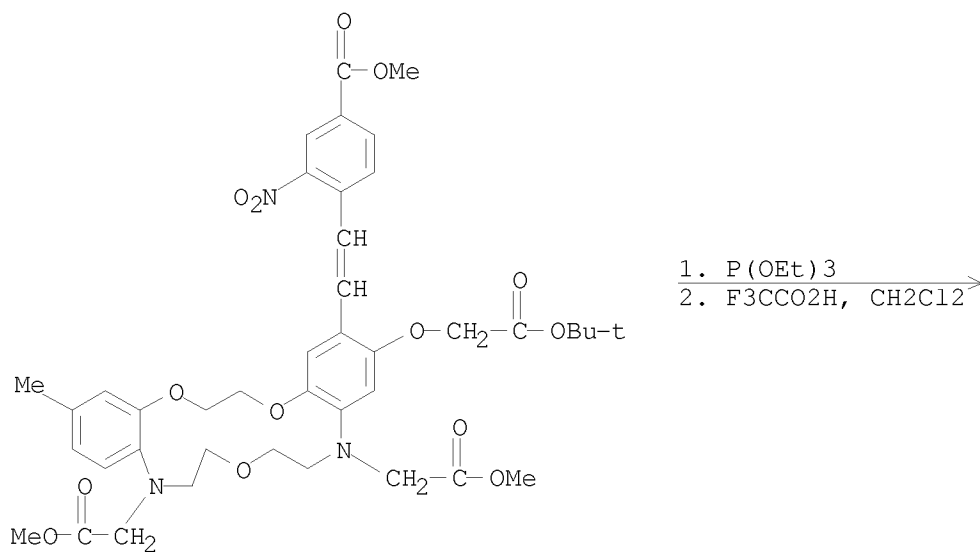
NOTE: 2) incremental addition of reagent in stage 1

CON: STEP(1) 6 hours, 120 deg C

STEP(2.1) 22 hours, room temperature

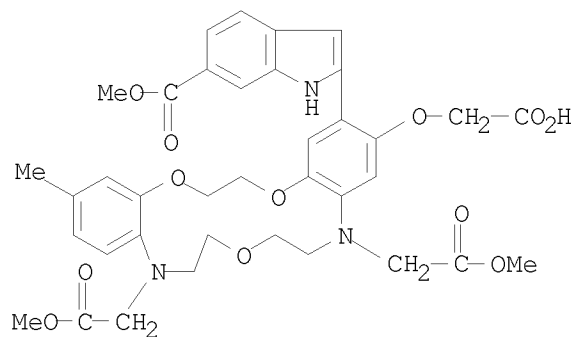
STEP(2.2) room temperature, pH 3

## RX(151) OF 555 - 2 STEPS





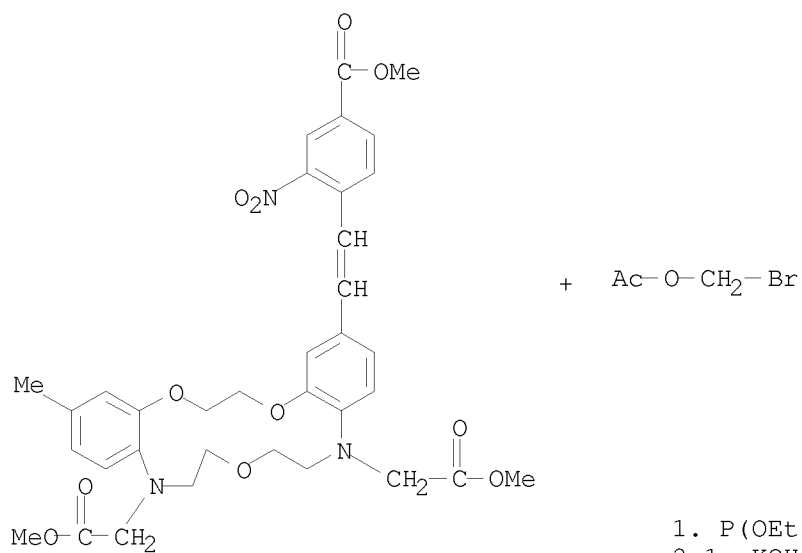
RX(151) OF 555 - 2 STEPS



57%

CON: STEP(1) 7 hours, 130 deg C  
STEP(2) 3 hours, room temperature

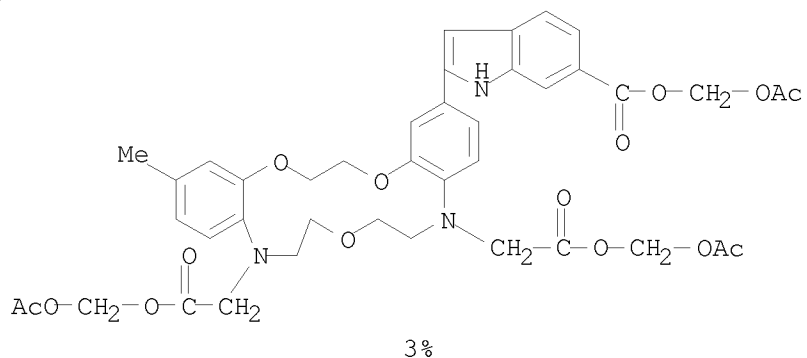
RX(270) OF 555 - 3 STEPS



+ Ac-O-CH<sub>2</sub>-Br

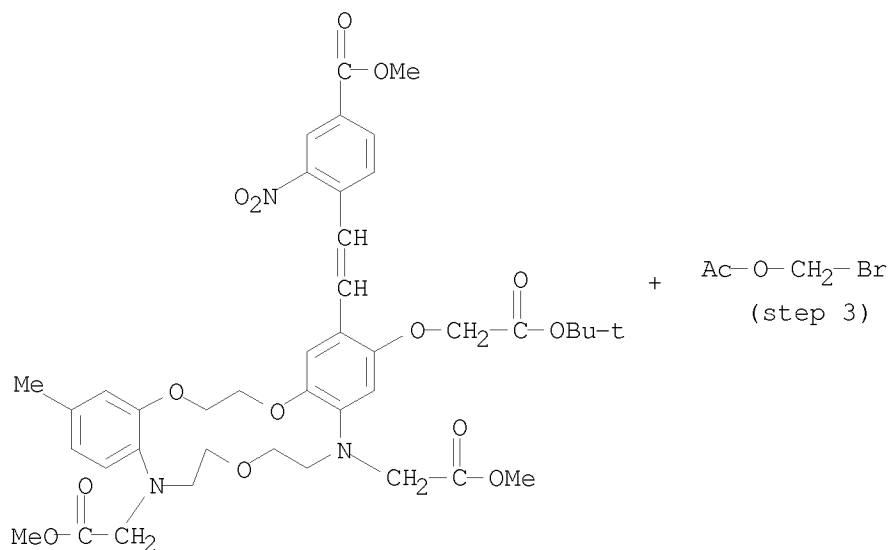
1. P(OEt)<sub>3</sub>  
2.1. KOH, Water, MeOH  
2.2. HCl, Water  
3.1. EtN(Pr-i)<sub>2</sub>, DMF  
3.2. AcOH, Water

## RX(270) OF 555 - 3 STEPS



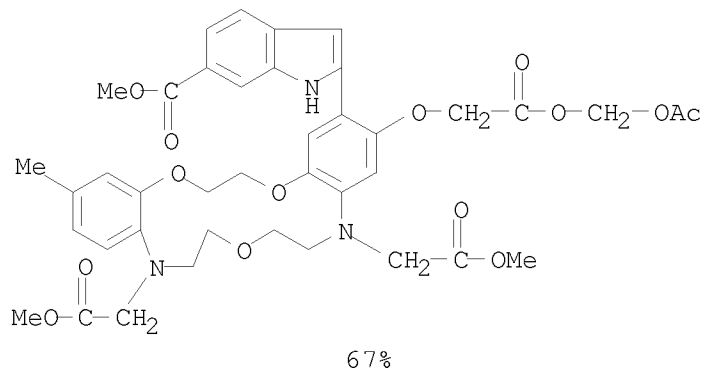
NOTE: 2) incremental addition of reagent in stage 1  
CON: STEP(1) 6 hours, 120 deg C  
STEP(2.1) 22 hours, room temperature  
STEP(2.2) room temperature, pH 3  
STEP(3.1) 16 hours, room temperature  
STEP(3.2) room temperature

## RX(300) OF 555 - 3 STEPS



1.  $\text{P}(\text{OEt})_3$
2.  $\text{F}_3\text{CCO}_2\text{H}$ ,  $\text{CH}_2\text{Cl}_2$
3.  $\text{EtN}(\text{Pr-}i)_2$ ,  $\text{DMF}$

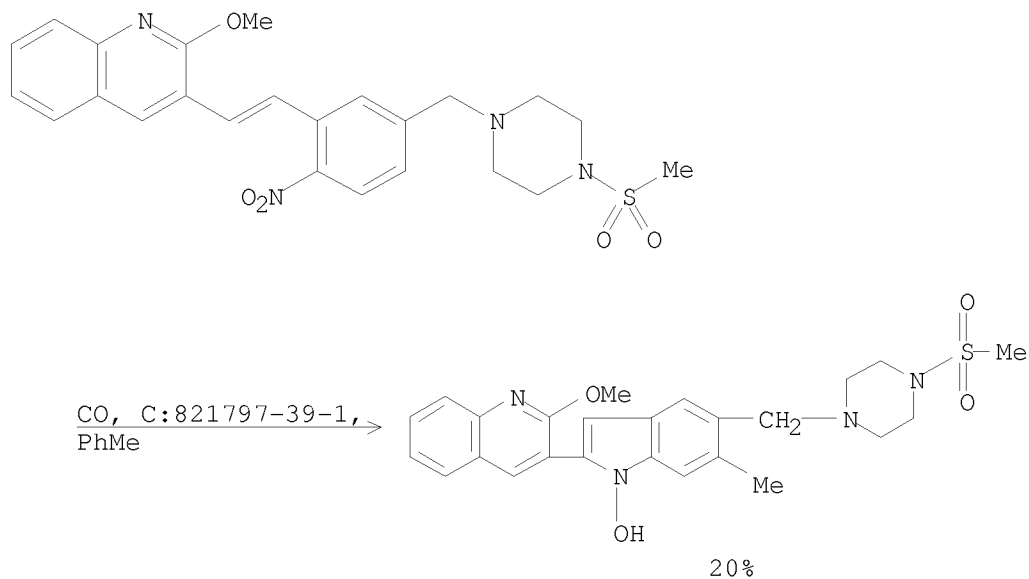
RX(300) OF 555 - 3 STEPS



CON: STEP(1) 7 hours, 130 deg C  
 STEP(2) 3 hours, room temperature  
 STEP(3) 16 hours, room temperature

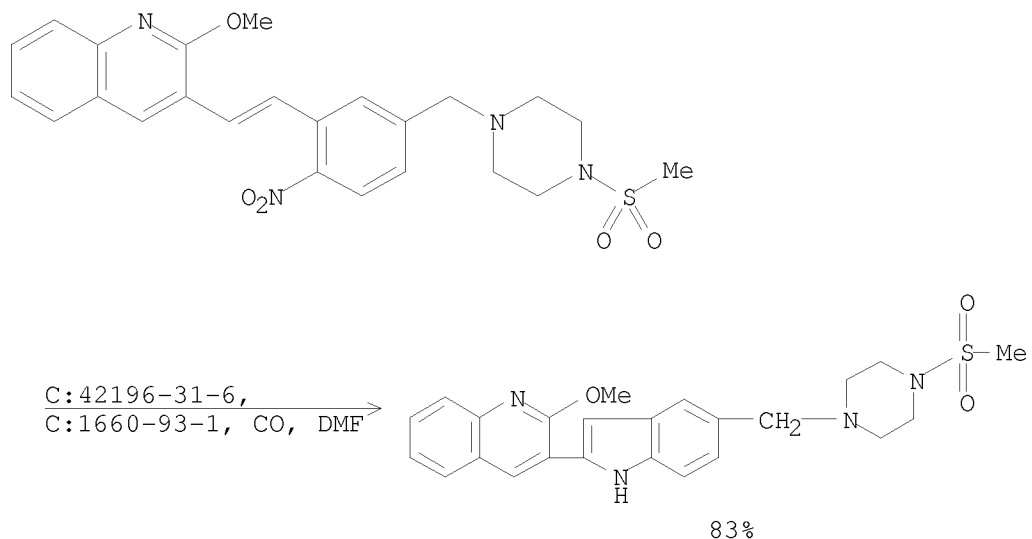
L4 ANSWER 7 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(5) OF 30



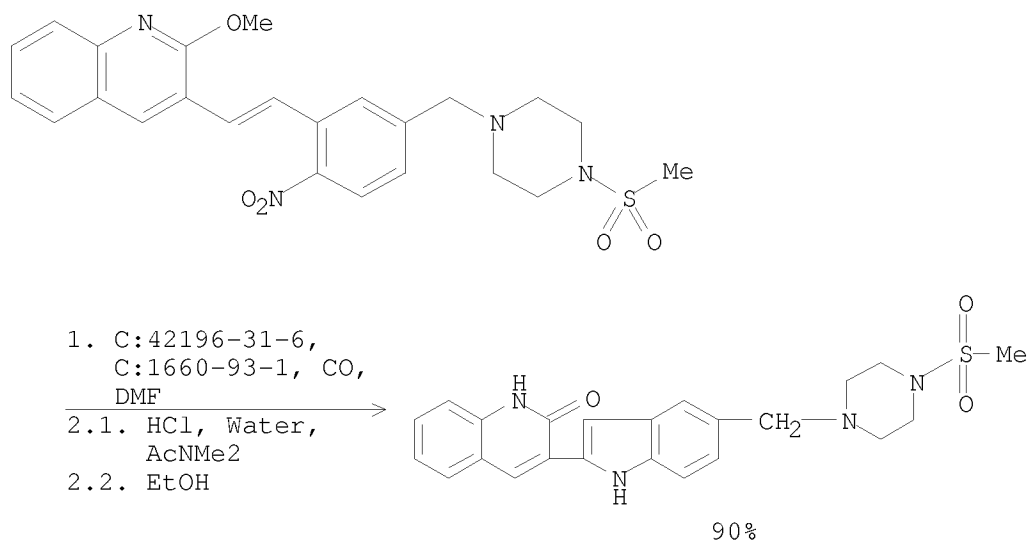
NOTE: Endeavor reactor was used  
 CON: STAGE(1) room temperature, 15 psi; 16 hours, 70 deg C

RX(6) OF 30



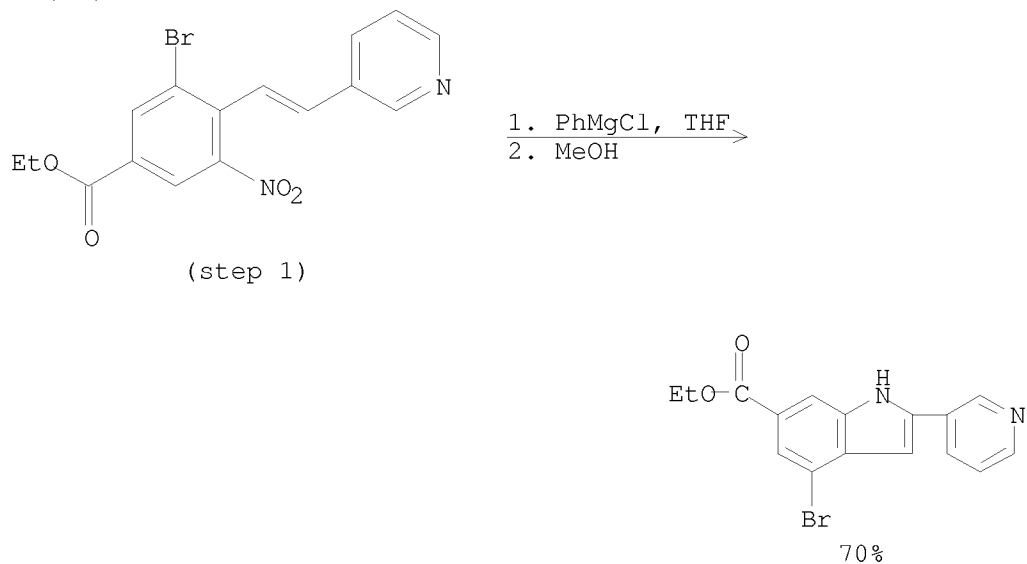
CON: STAGE(1) room temperature, 15 psi; 14 hours, 70 deg C

RX(13) OF 30 - 2 STEPS



CON: STEP(1.1) room temperature, 15 psi; 14 hours, 70 deg C  
STEP(2.1) 2 hours; 60 deg C

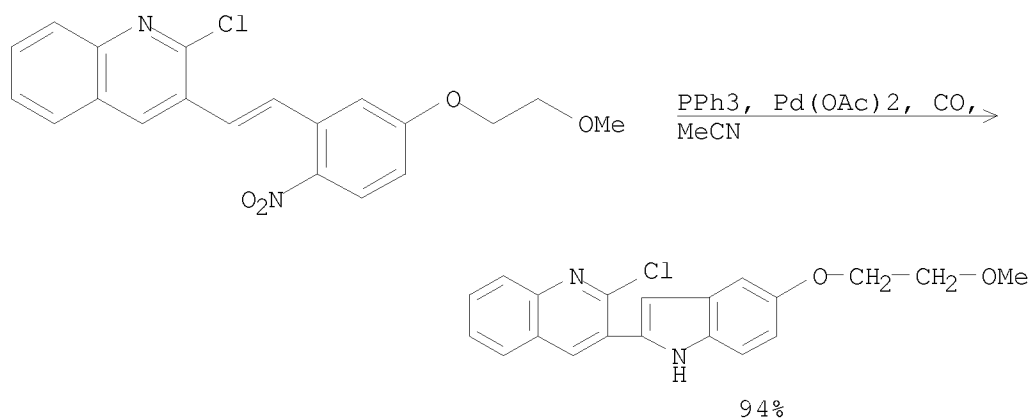
RX(37) OF 85



CON: 30 minutes, -40 deg C

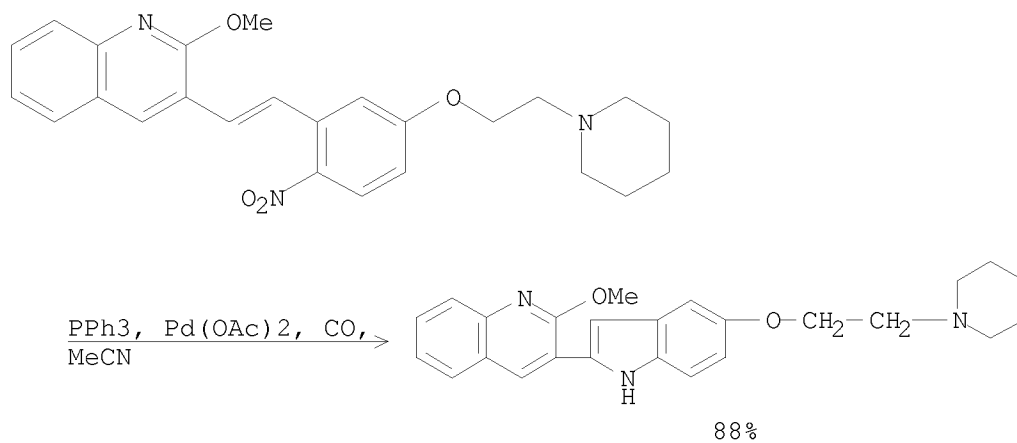
L4 ANSWER 9 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(4) OF 63



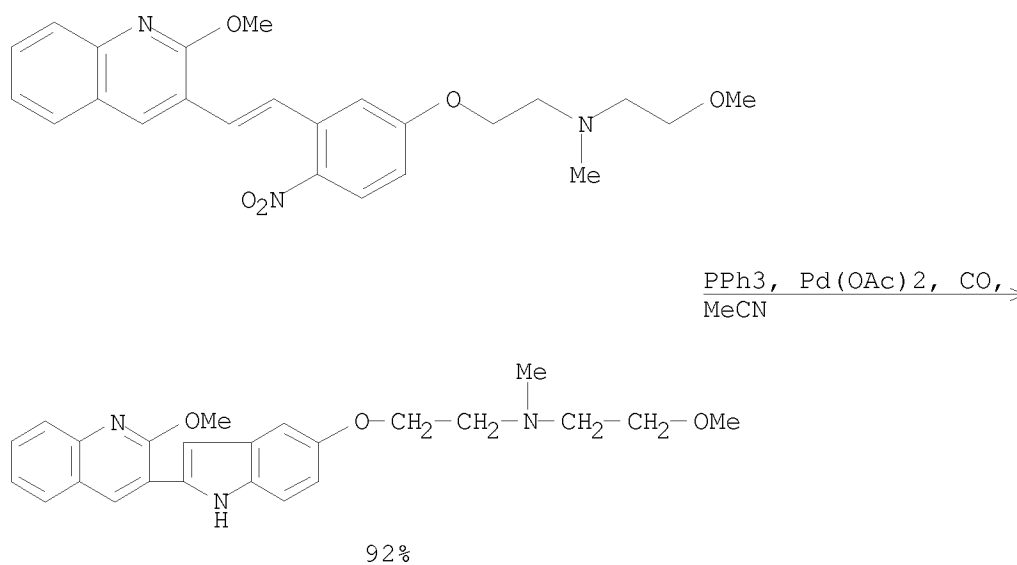
NOTE: alternative prepn. shown  
 CON: 12 hours, 70 deg C, 6 atm

RX(10) OF 63



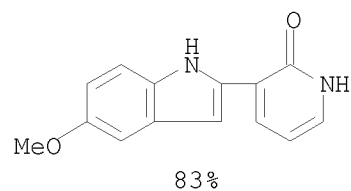
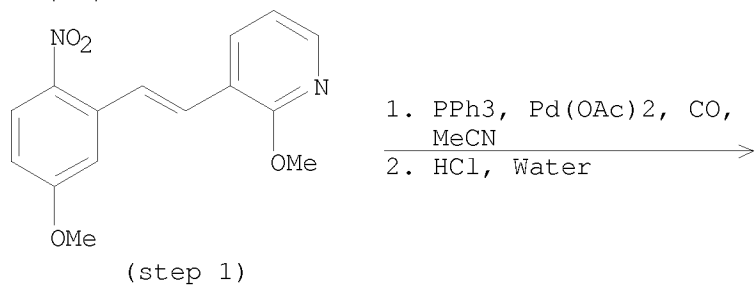
NOTE: alternative prepn. shown  
 CON: 12 hours, 70 deg C, 6 atm

RX(15) OF 63



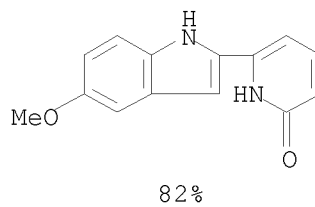
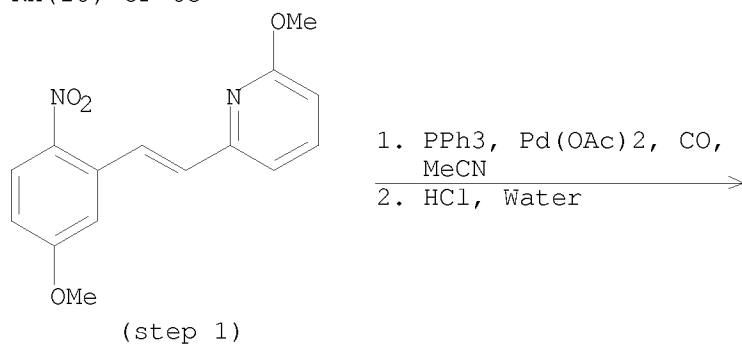
NOTE: alternative prepn. shown  
 CON: 12 hours, 70 deg C, 6 atm

RX(17) OF 63



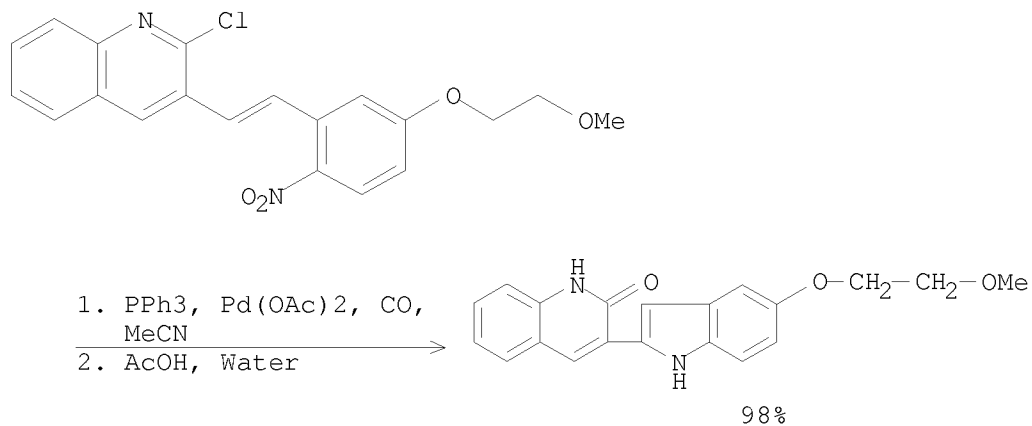
CON: STAGE(1) 12 hours, 70 deg C, 6 atm  
STAGE(2) 12 hours, reflux

RX(18) OF 63



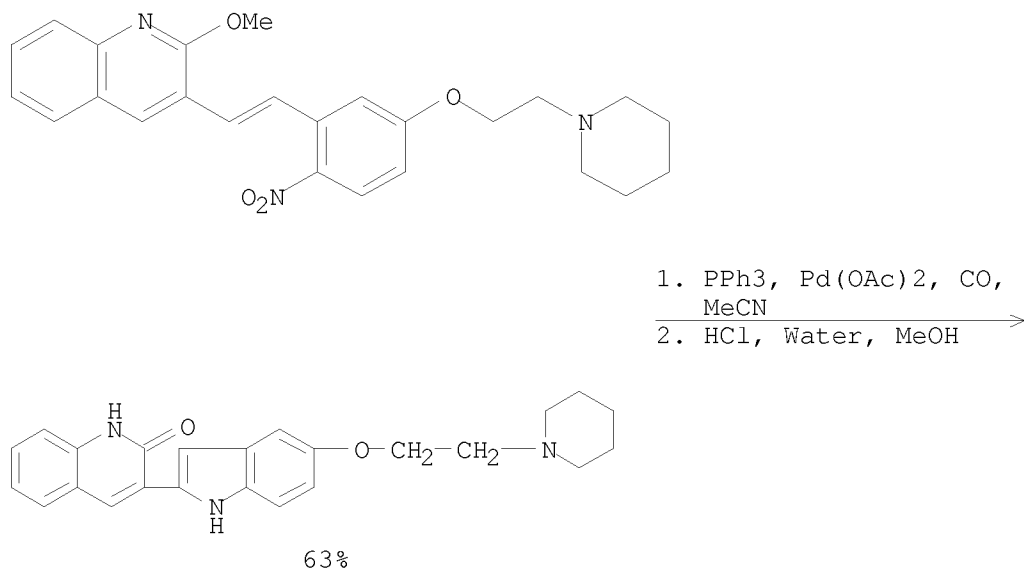
CON: STAGE(1) 12 hours, 70 deg C, 6 atm  
STAGE(2) 12 hours, reflux

RX(25) OF 63 - 2 STEPS



NOTE: 1) alternative prepn. shown, 2) alternative prepn. shown  
 CON: STEP(1) 12 hours, 70 deg C, 6 atm  
 STEP(2) 3 hours, reflux

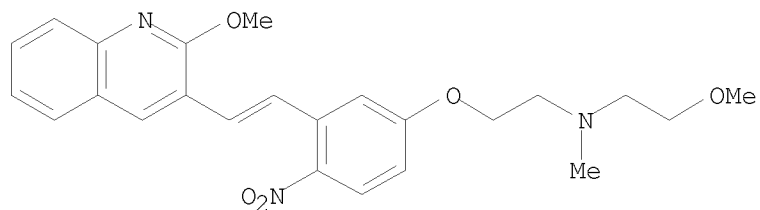
RX(29) OF 63 - 2 STEPS



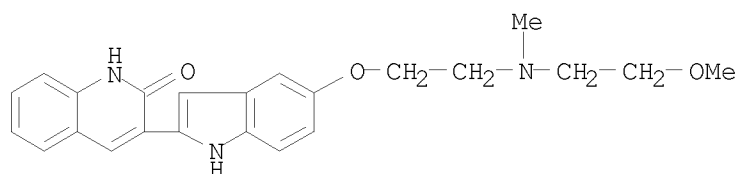
NOTE: 1) alternative prepn. shown  
 CON: STEP(1) 12 hours, 70 deg C, 6 atm  
 STEP(2) 4 hours, reflux



RX(33) OF 63 - 2 STEPS



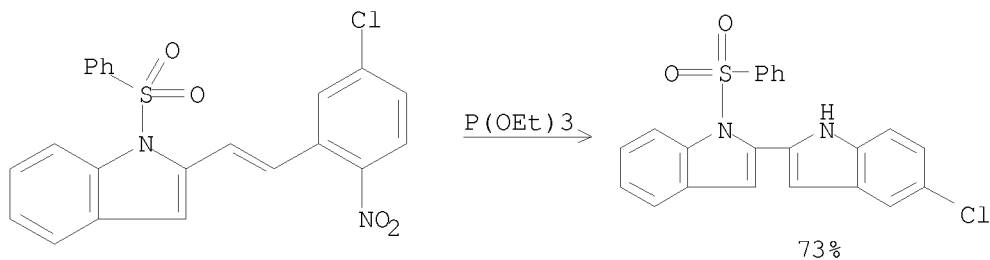
1. PPh<sub>3</sub>, Pd(OAc)<sub>2</sub>, CO,  
MeCN  
2. HCl, Water, MeOH →



NOTE: 1) alternative prepn. shown  
CON: STEP(1) 12 hours, 70 deg C, 6 atm  
STEP(2) 4 hours, reflux

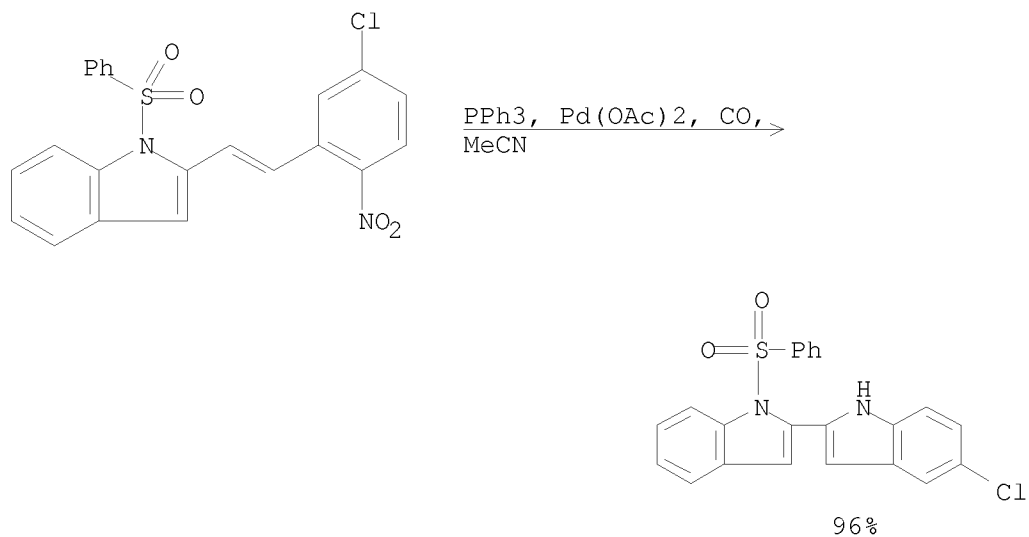
L4 ANSWER 10 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(3) OF 71



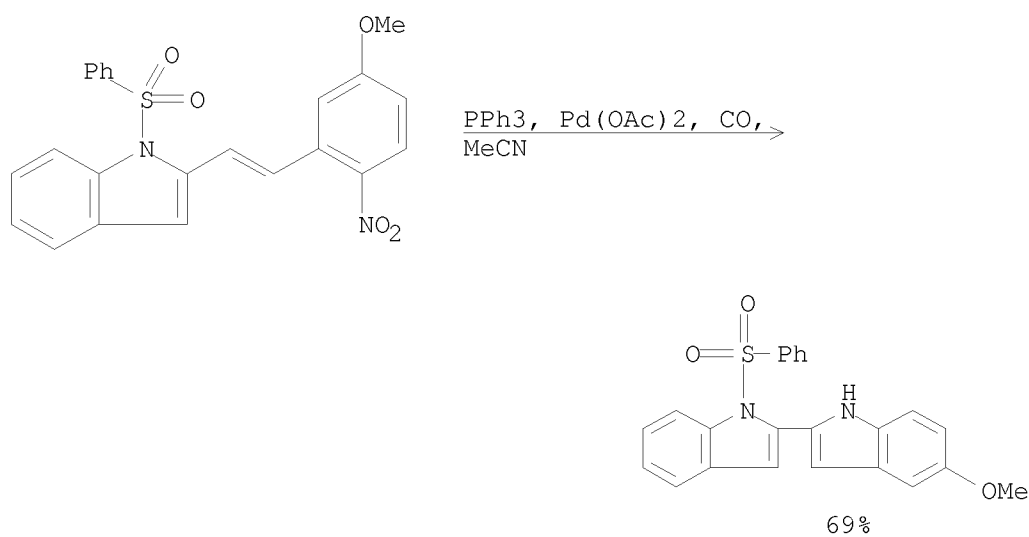
CON: 2 hours, 155 deg C

RX(4) OF 71



CON: 12 hours, 70 deg C

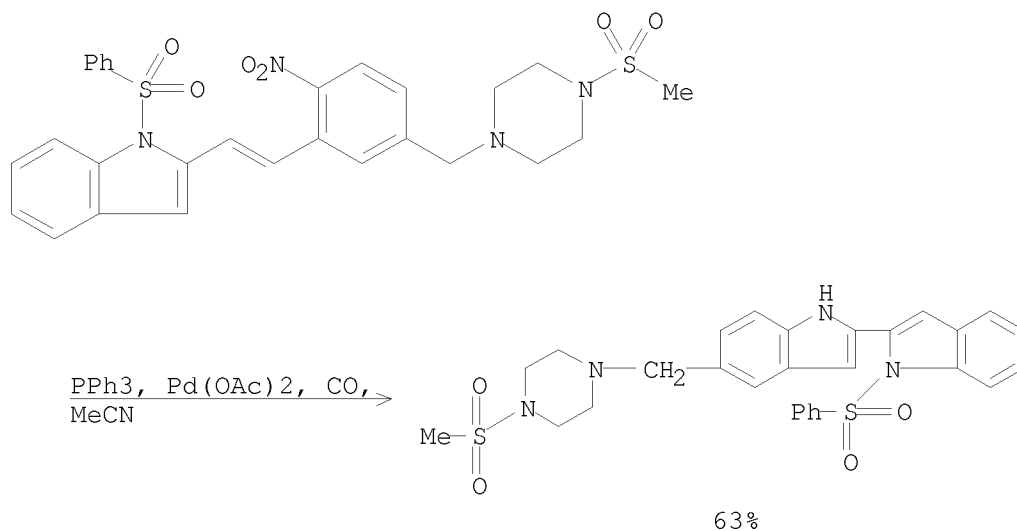
RX(6) OF 71



NOTE: using other method also got good yield

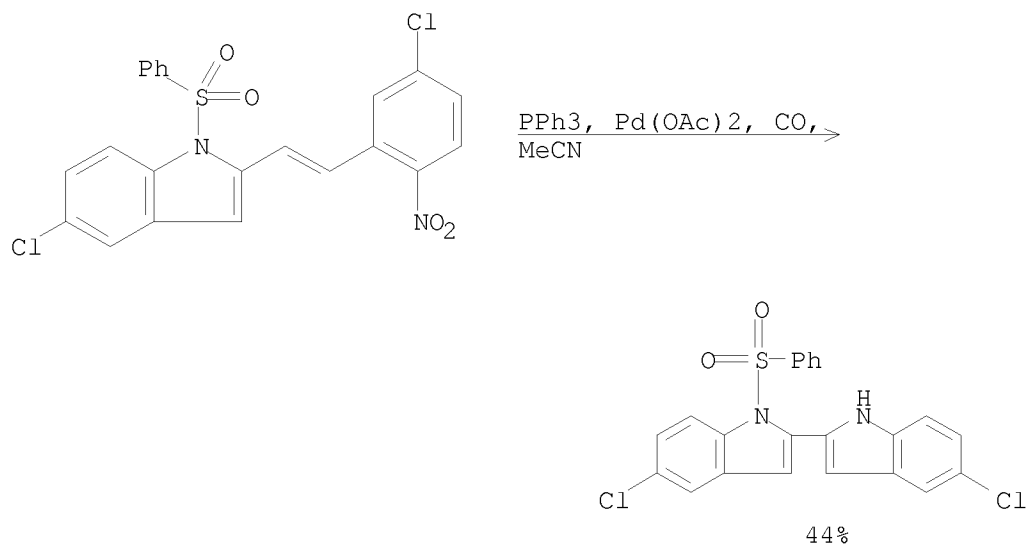
CON: 12 hours, 70 deg C

RX(7) OF 71



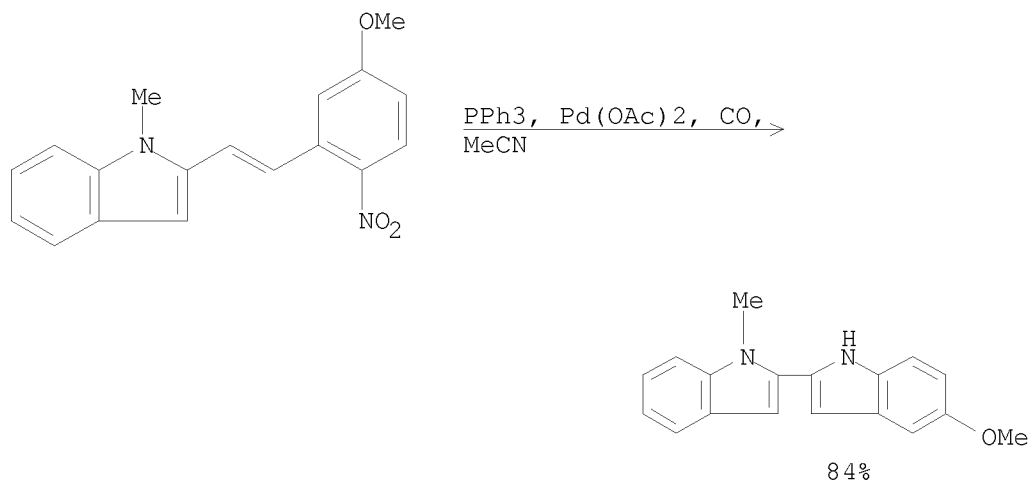
NOTE: using other method also got good yield  
CON: 12 hours, 70 deg C

RX(9) OF 71



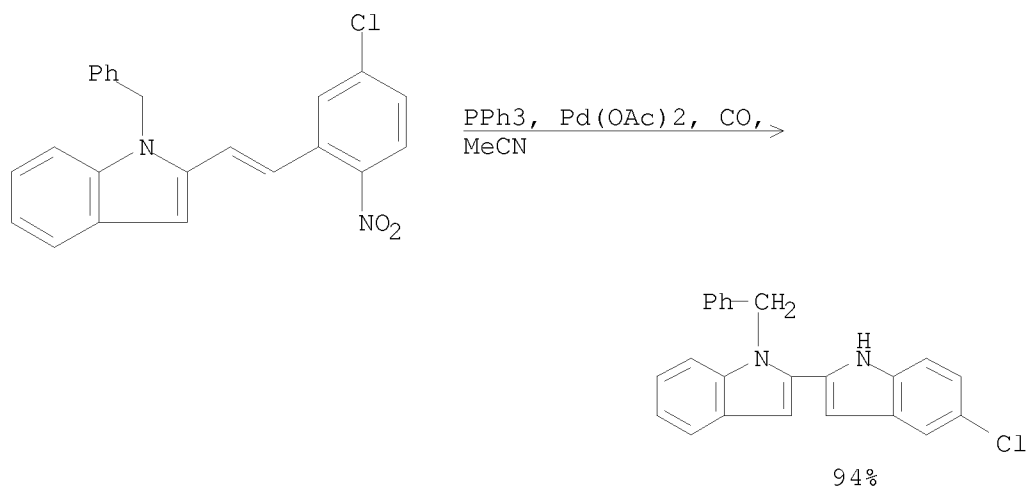
NOTE: using other method also got good yield  
CON: 12 hours, 70 deg C

RX(11) OF 71



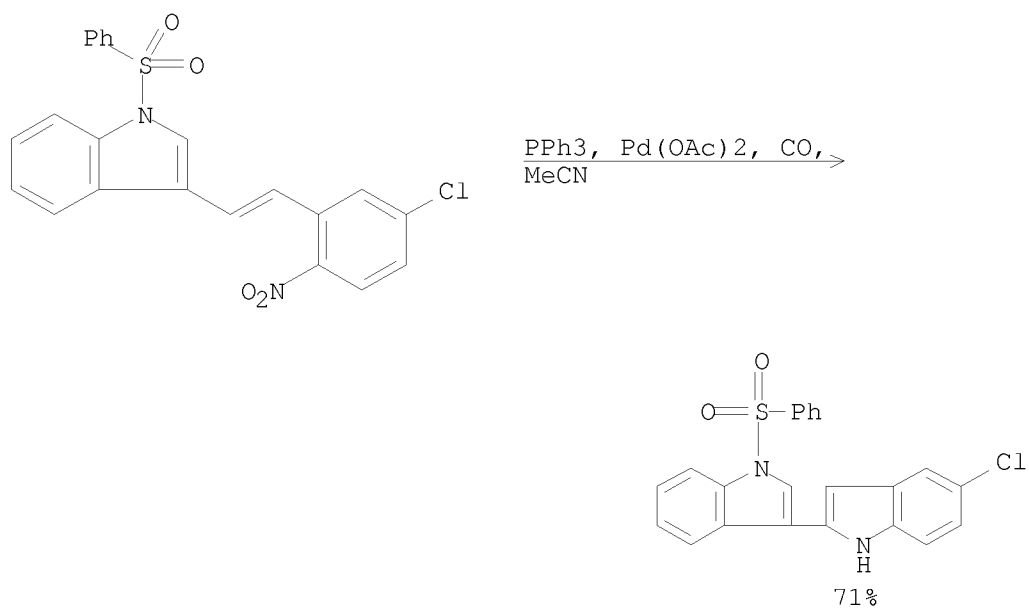
NOTE: using other method also got good yield  
 CON: 12 hours, 70 deg C

RX(14) OF 71



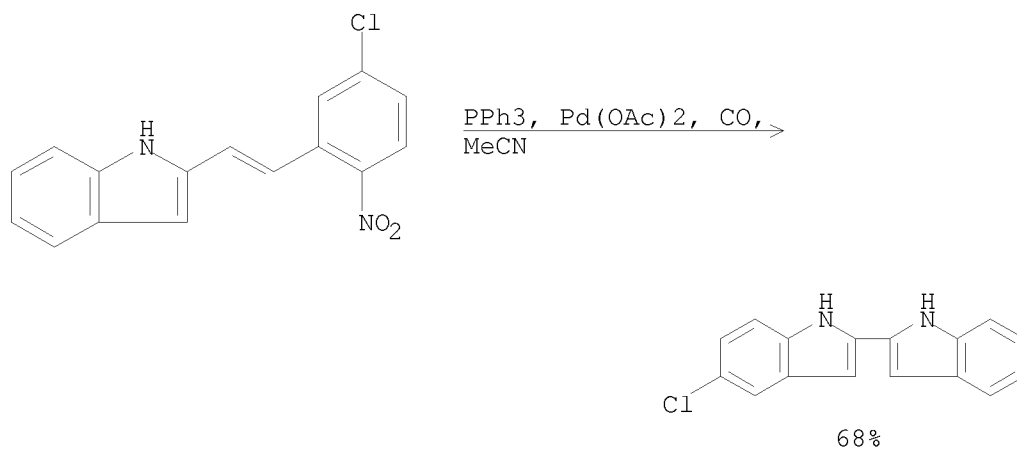
NOTE: using other method also got good yield  
 CON: 12 hours, 70 deg C

RX(16) OF 71



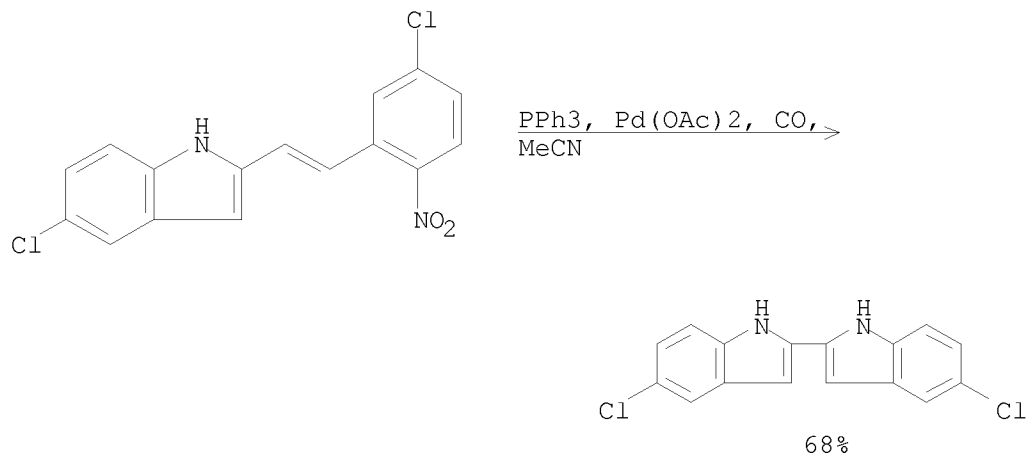
NOTE: using other method also got good yield  
 CON: 12 hours, 70 deg C

RX(18) OF 71



NOTE: using other method also got good yield  
 CON: 12 hours, 70 deg C

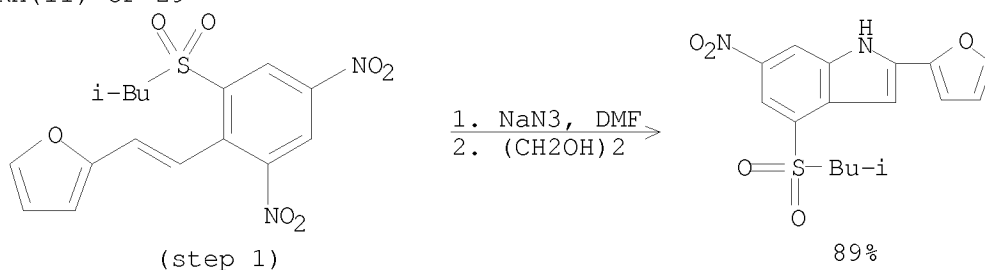
RX(21) OF 71



NOTE: using other method also got good yield  
 CON: 12 hours, 70 deg C

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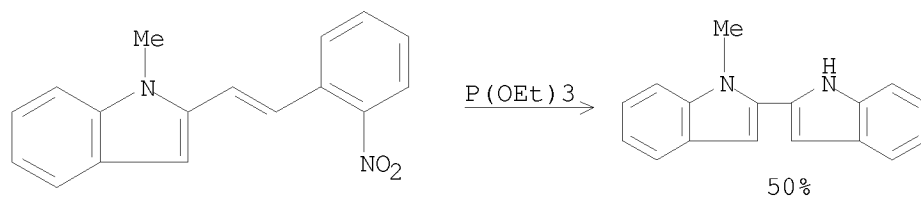
RX(11) OF 29



NOTE: regioselective, thermal, stereoselective

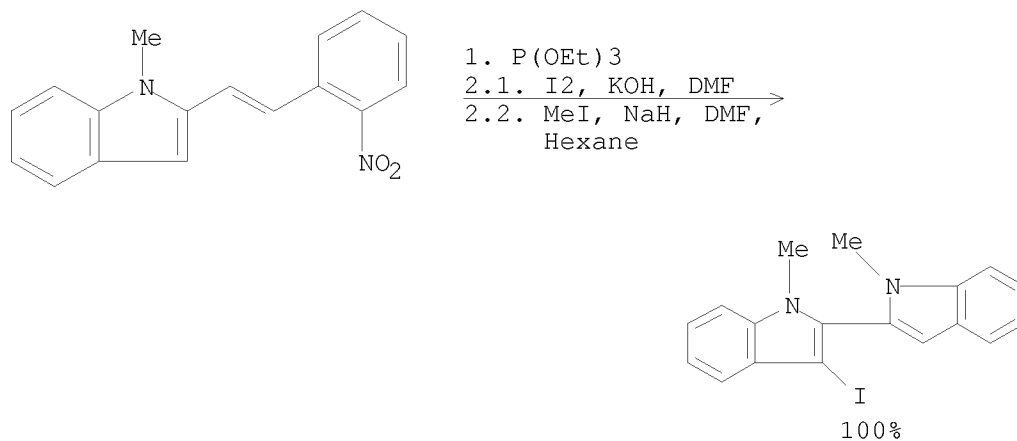
L4 ANSWER 12 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(10) OF 177



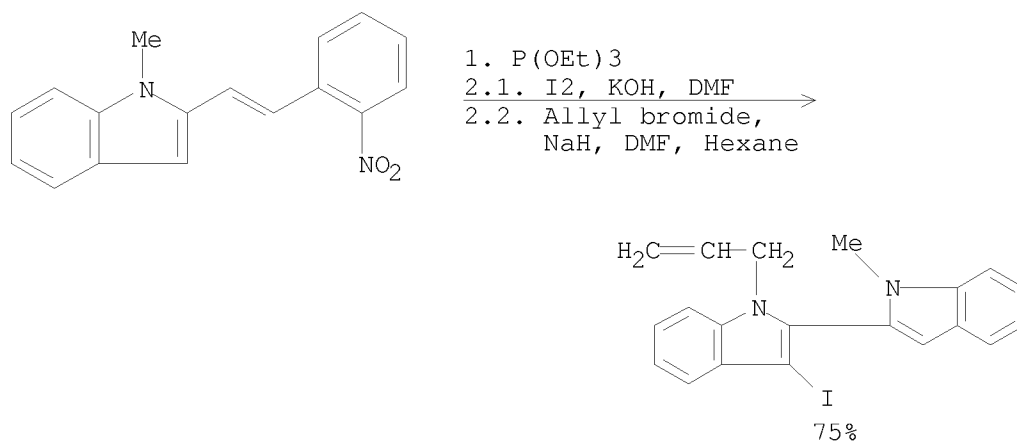
NOTE: thermal, alternative preps. gave similar yields

RX(43) OF 177 - 2 STEPS



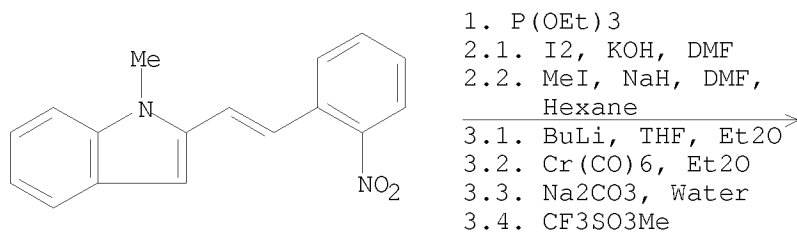
NOTE: 1) thermal, alternative preps. gave similar yields

RX(44) OF 177 - 2 STEPS

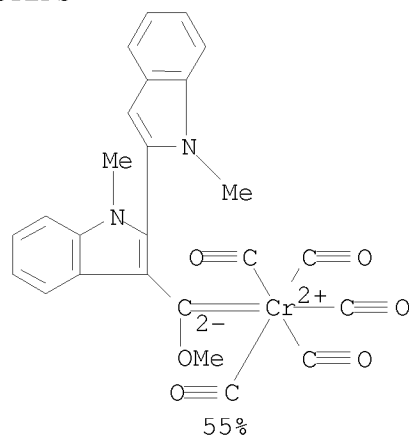


NOTE: 1) thermal, alternative preps. gave similar yields, 2) reactant assumed

RX(79) OF 177 - 3 STEPS

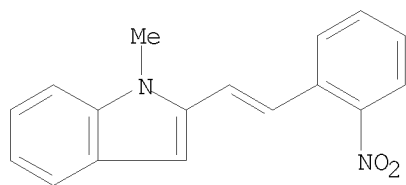


RX(79) OF 177 - 3 STEPS

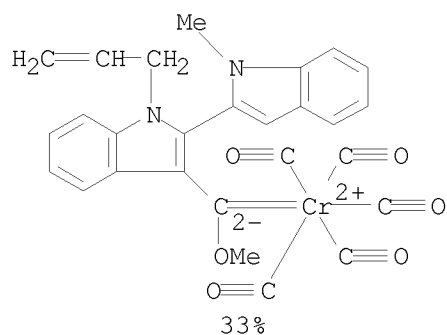


NOTE: 1) thermal, alternative preps. gave similar yields

RX(80) OF 177 - 3 STEPS



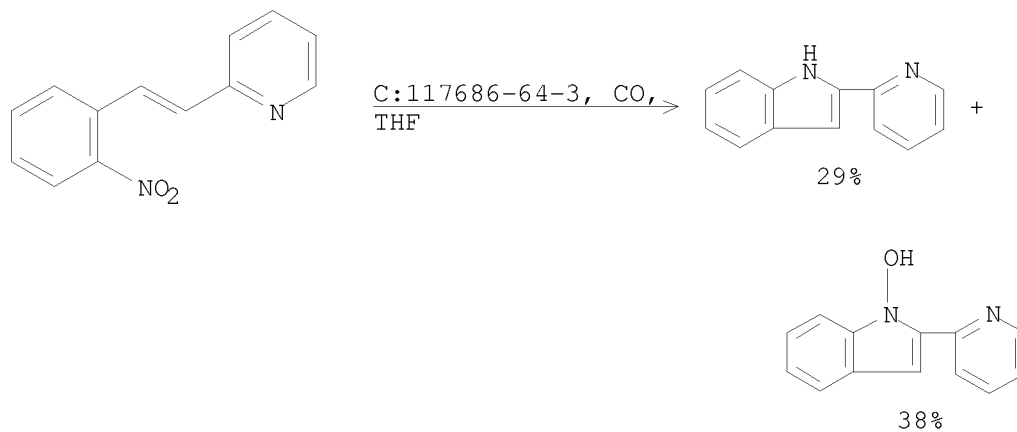
1. P(OEt)<sub>3</sub>
- 2.1. I<sub>2</sub>, KOH, DMF
- 2.2. Allyl bromide,  
NaH, DMF, Hexane
- 3.1. BuLi, THF, Et<sub>2</sub>O
- 3.2. Cr(CO)<sub>6</sub>, Et<sub>2</sub>O
- 3.3. Na<sub>2</sub>CO<sub>3</sub>, Water
- 3.4. CF<sub>3</sub>SO<sub>3</sub>Me



NOTE: 1) thermal, alternative preps. gave similar yields, 2) reactant assumed

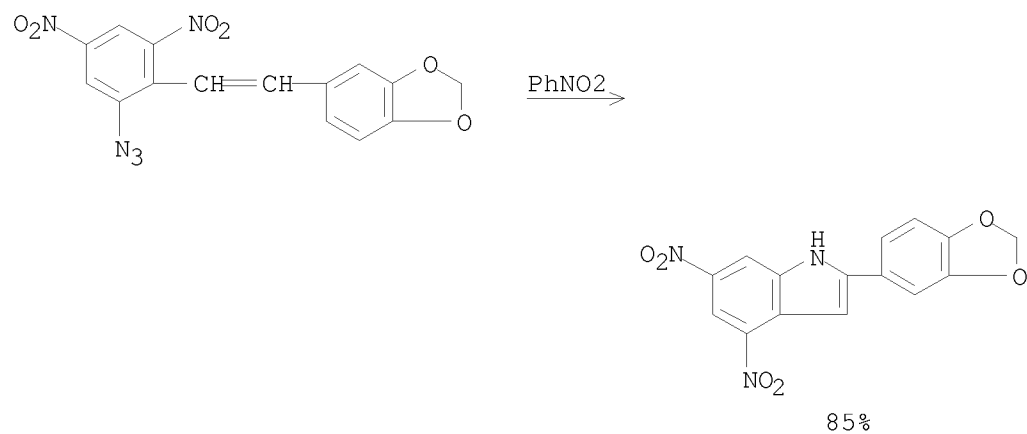


RX(4) OF 5

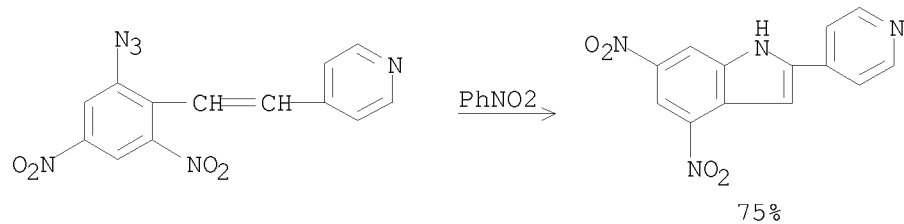


L4 ANSWER 14 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

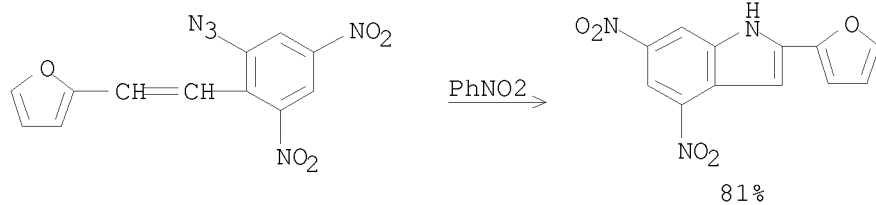
RX(22) OF 57



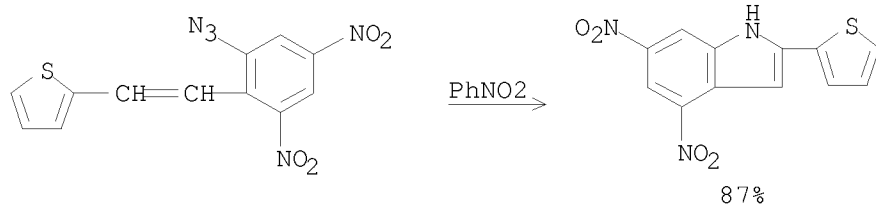
RX(24) OF 57



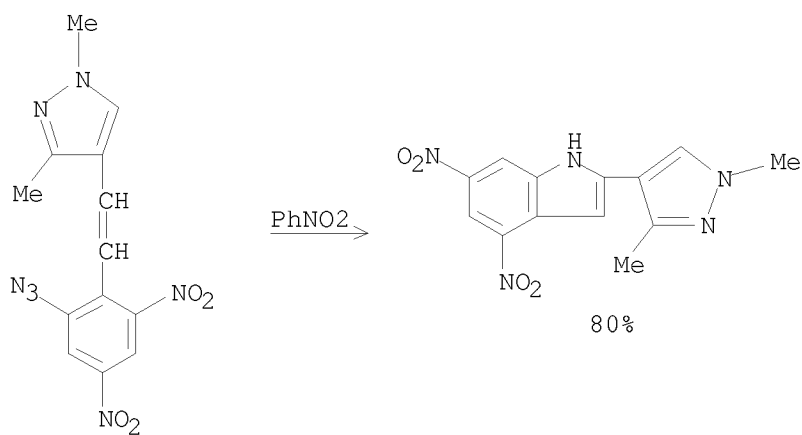
RX(25) OF 57



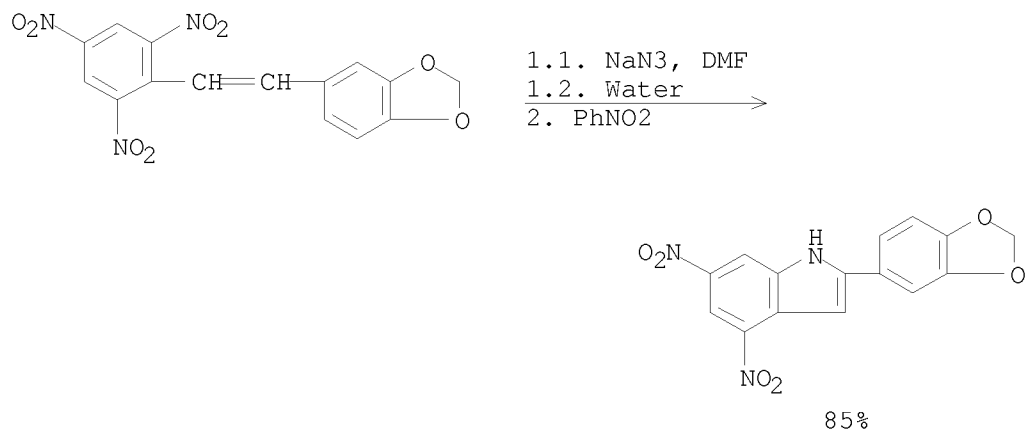
RX(26) OF 57



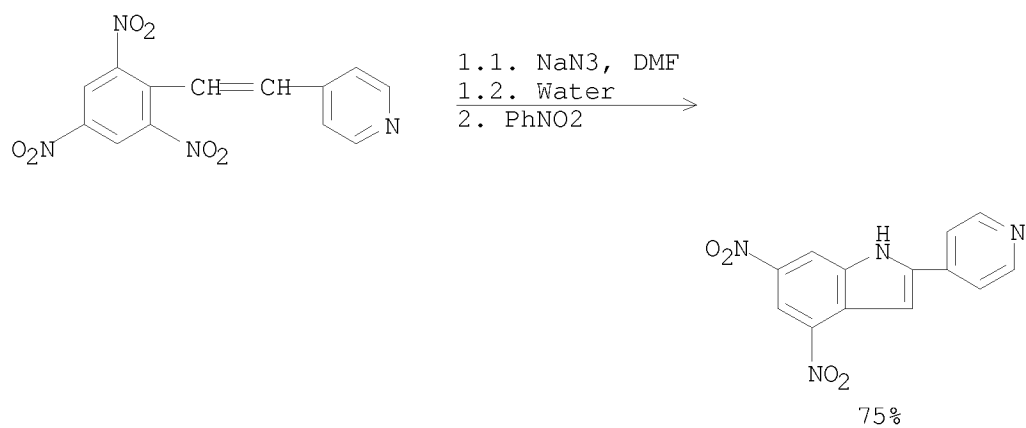
RX(28) OF 57



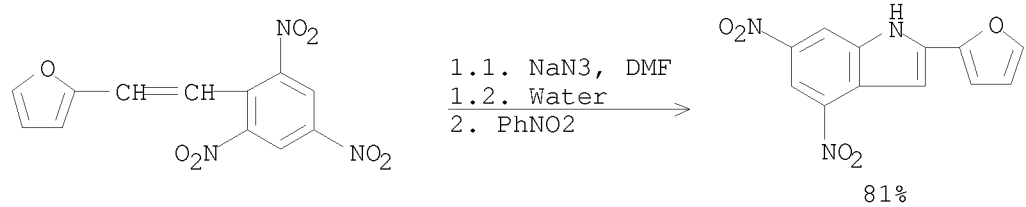
RX(41) OF 57 - 2 STEPS



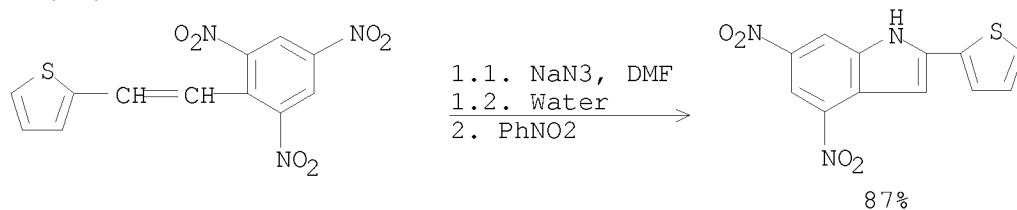
RX(43) OF 57 - 2 STEPS



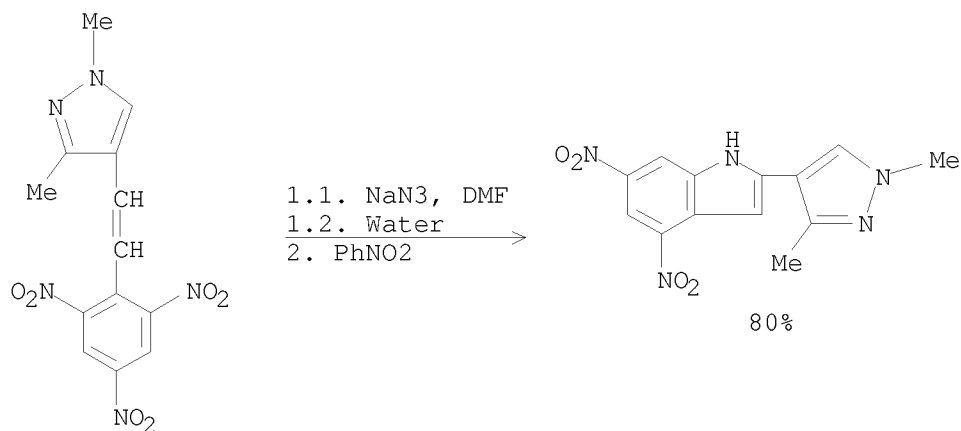
RX(44) OF 57 - 2 STEPS



RX(45) OF 57 - 2 STEPS

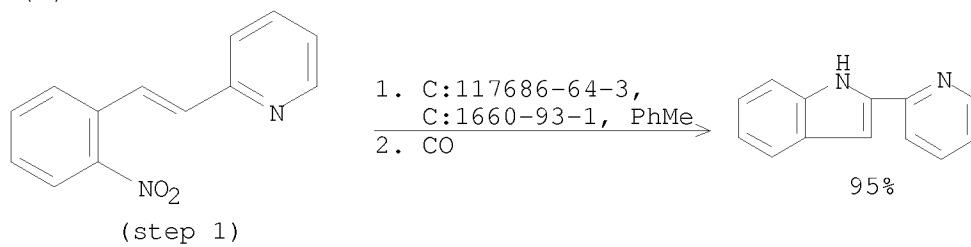


RX(47) OF 57 - 2 STEPS

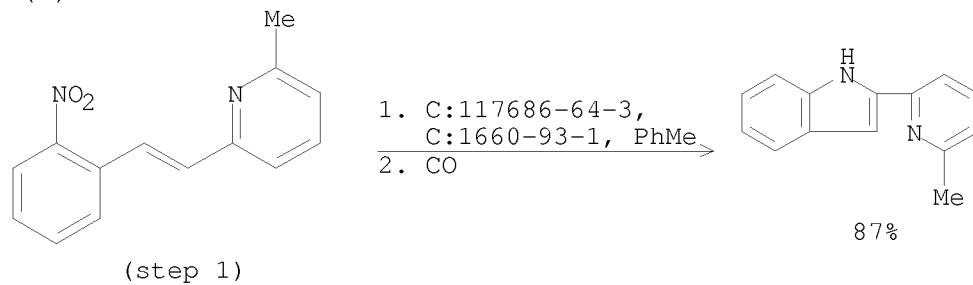


L4 ANSWER 15 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

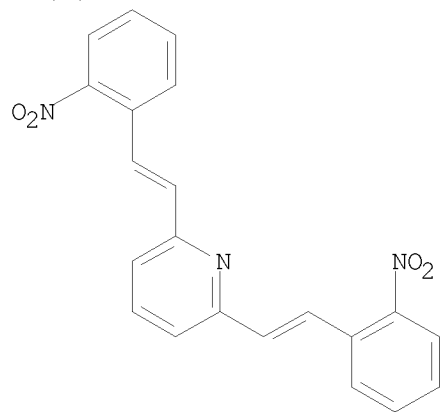
RX(1) OF 9



RX(2) OF 9

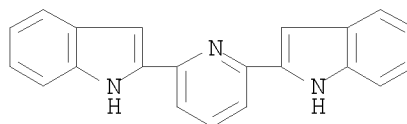


RX(3) OF 9



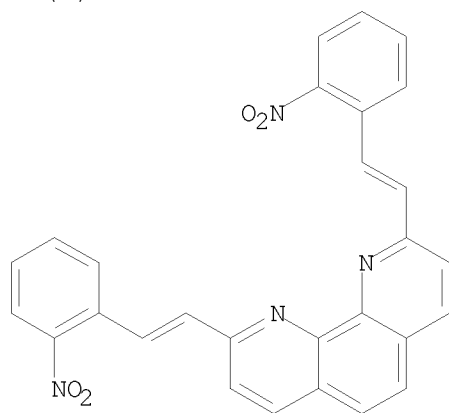
(step 1)

1. C:117686-64-3,  
C:1660-93-1, PhMe  
2. CO



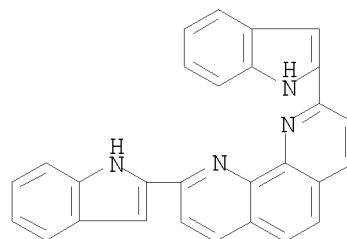
56%

RX(4) OF 9



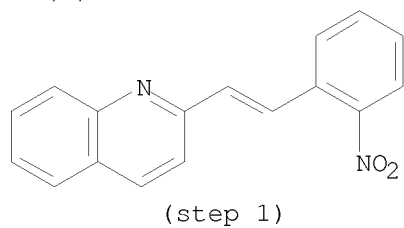
(step 1)

1. C:117686-64-3,  
C:1660-93-1, PhMe  
2. CO

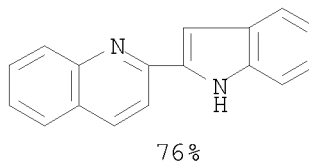


65%

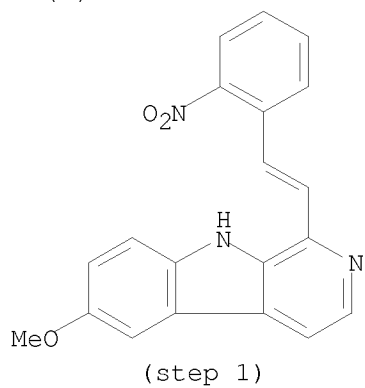
RX(5) OF 9



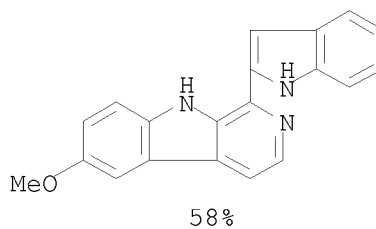
1. C:117686-64-3,  
C:1660-93-1, PhMe  
2. CO



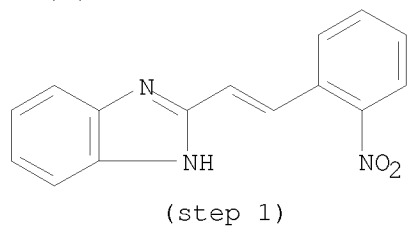
RX(6) OF 9



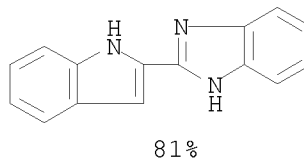
1. C:117686-64-3,  
C:1660-93-1, PhMe  
2. CO



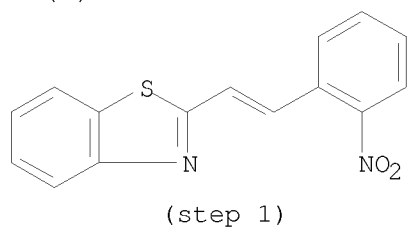
RX(7) OF 9



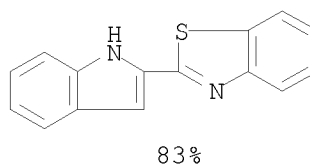
1. C:117686-64-3,  
C:1660-93-1, PhMe  
2. CO



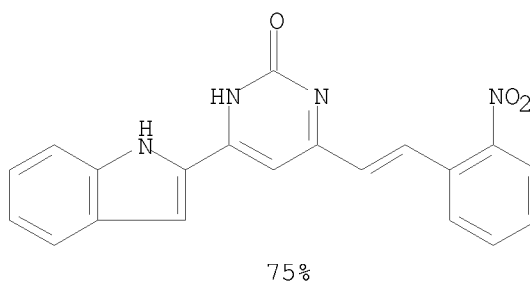
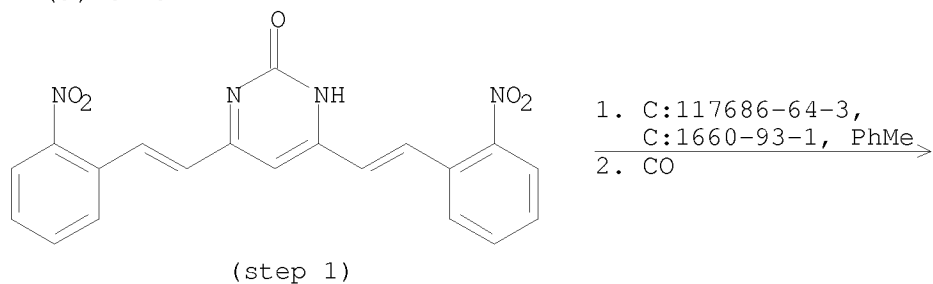
RX(8) OF 9



1. C:117686-64-3,  
C:1660-93-1, PhMe  
2. CO

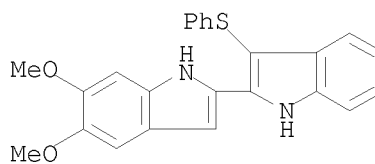
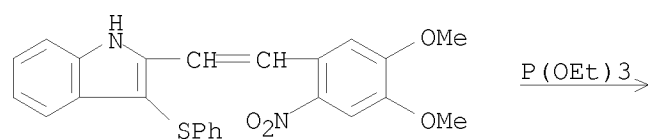


RX(9) OF 9

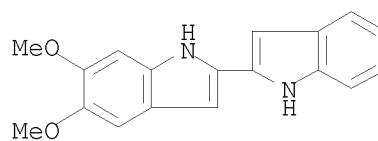
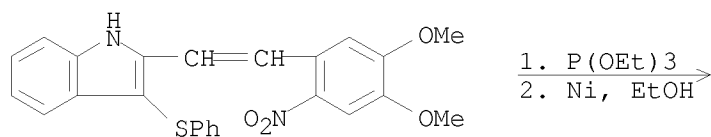


L4 ANSWER 16 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(2) OF 6



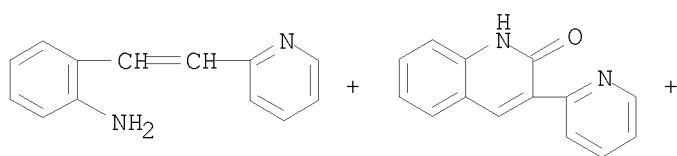
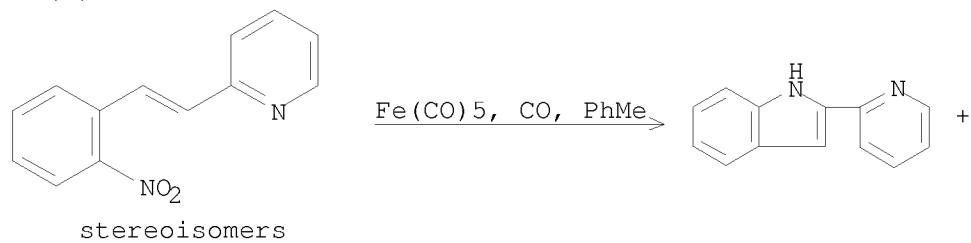
RX(5) OF 6 - 2 STEPS



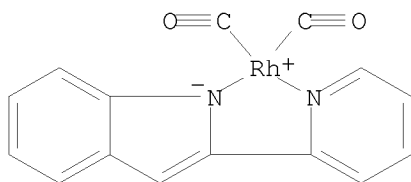


L4 ANSWER 17 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

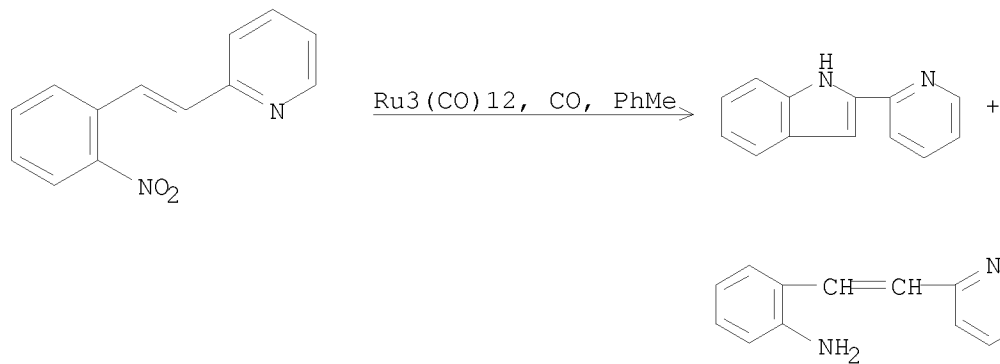
RX(8) OF 12



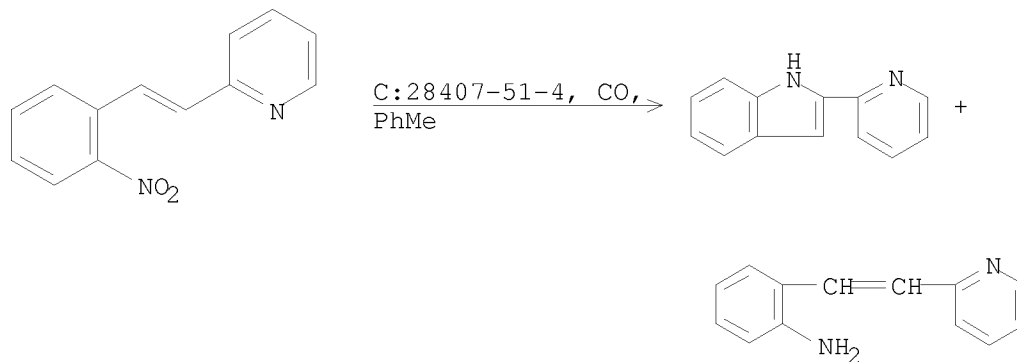
RX(8) OF 12



RX(9) OF 12

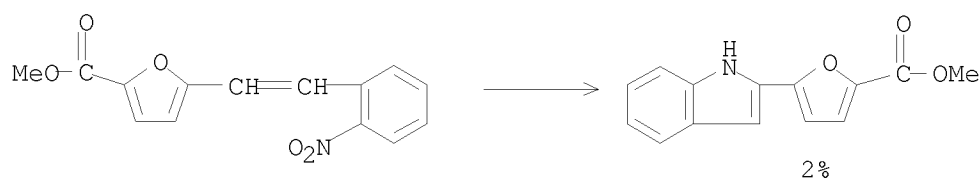


RX(10) OF 12

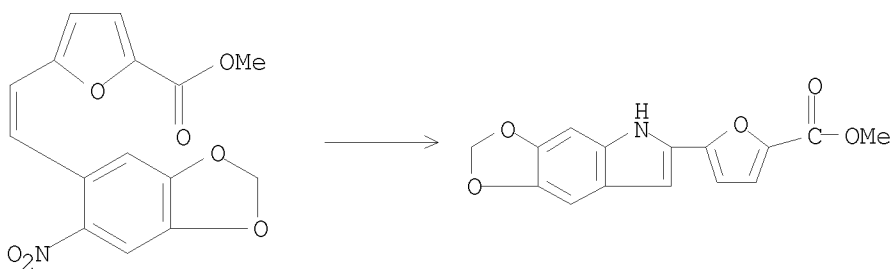


L4 ANSWER 18 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

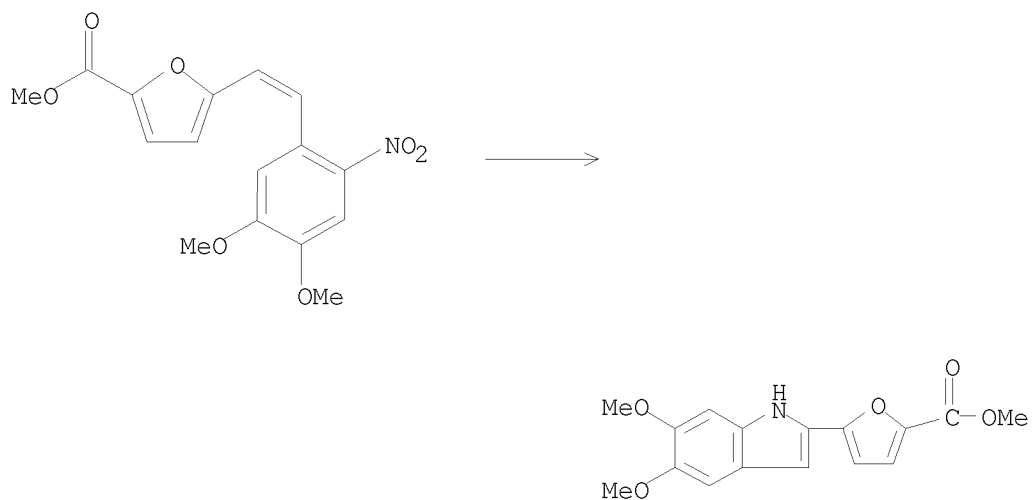
RX(69) OF 98 - 3 STEPS



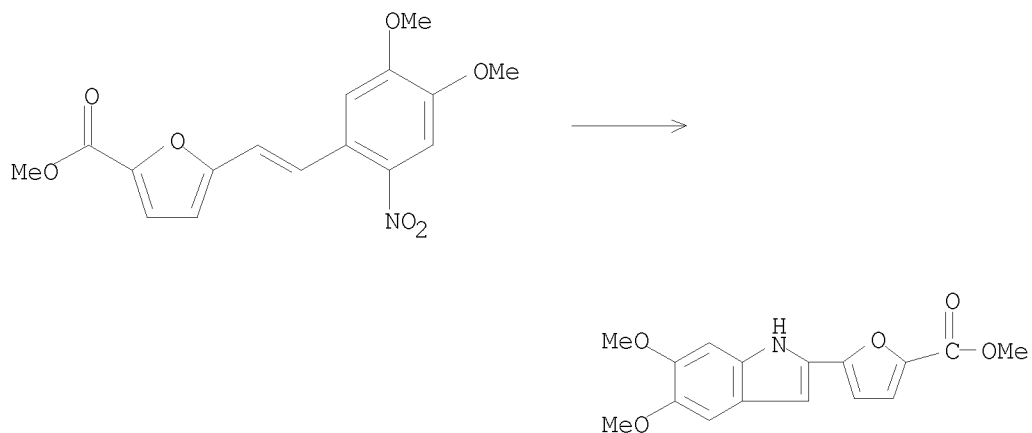
RX(72) OF 98 - 3 STEPS



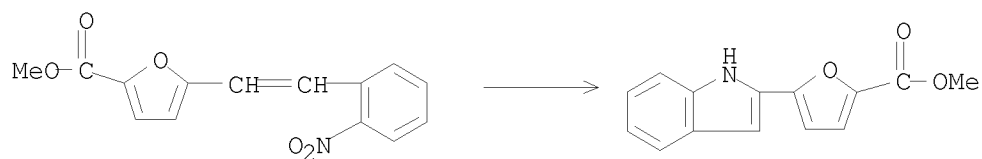
RX(73) OF 98 - 3 STEPS



RX(76) OF 98 - 3 STEPS



RX(80) OF 98 - 4 STEPS



=> d 1-18 crdef abs  
'CRDEF' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS ----- GI and AB  
 ALL ----- BIB, AB, IND, RE, Single-step Reactions  
 APPS ----- AI, PRAI  
 BIB ----- AN, plus Bibliographic Data  
 CAN ----- List of CA abstract numbers without answer numbers  
 CBIB ----- AN, plus Compressed Bibliographic Data  
 DALL ----- ALL, delimited (end of each field identified)  
 IABS ----- ABS, indented with text labels  
 IALL ----- ALL, indented with text labels  
 IBIB ----- BIB, indented with text labels  
 IND ----- Indexing data  
 IPC ----- International Patent Classifications  
 ISTD ----- STD, indented with text labels  
 OBIB ----- AN, plus Bibliographic Data (original)  
 OIBIB ----- OBIB, indented with text labels  
  
 SBIB ----- BIB, no citations  
 SIBIB ----- IBIB, no citations  
  
 MAX ----- Same as ALL  
 PATS ----- PI, SO  
 SCAN ----- TI and FCRD (random display, no answer number. SCAN  
                   must be entered on the same line as DISPLAY, e.g.,  
                   D SCAN.)  
 SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for  
                   all single-step reactions)  
 STD ----- BIB, IPC, and NCL  
  
 CRD ----- Compact Display of All Hit Reactions  
 CRDREF ----- Compact Reaction Display and SO, PY for Reference  
 FHIT ----- Reaction Map, Diagram, and Summary for first  
                   hit reaction  
 FHITCBIB --- FHIT, AN plus CBIB  
 FCRD ----- First hit in Compact Reaction Display (CRD) format  
 FCRDREF ----- First hit in Compact Reaction Display (CRD) format with  
                   CA reference information (SO, PY). (Default)  
 FPATH ----- PATH, plus Reaction Summary for the "long path"  
 FSPATH ----- SPATH, plus Reaction Summary for the "short path"  
 HIT ----- Reaction Map, Reaction Diagram, and Reaction  
                   Summary for all hit reactions and fields containing  
                   hit terms  
 OCC ----- All hit fields and the number of occurrences of the  
                   hit terms in each field. Includes total number of  
                   HIT, PATH, SPATH reactions. Labels reactions that have  
                   incomplete verifications.  
 PATH ----- Reaction Map and Reaction Diagram for the "long  
                   path". Displays all hit reactions, except those  
                   whose steps are totally included within another hit  
                   reaction which is displayed  
 RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)  
 RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
 RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
 RXS ----- Hit Reaction Summaries (Map and Summary for all hit reactions)  
 SPATH ----- Reaction Map and Reaction Diagram for the "short  
                   path". Displays all single step reactions which

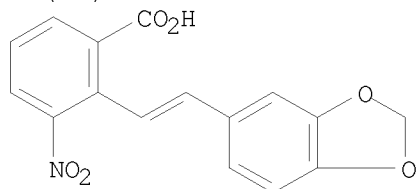
contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

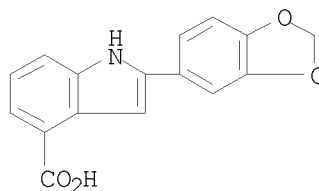
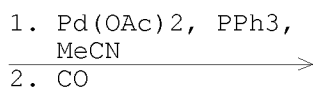
ENTER DISPLAY FORMAT (FCRDREF):crdref

L4 ANSWER 1 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(15) OF 47



(step 1)



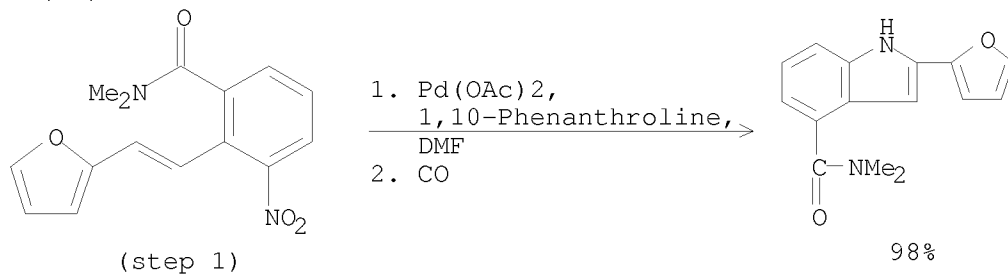
92%

REF: Tetrahedron, 62(49), 11381-11390; 2006

CON: STAGE(1) room temperature -> 70 deg C

STAGE(2) 16 hours, 70 deg C, 60 psi

RX(23) OF 47

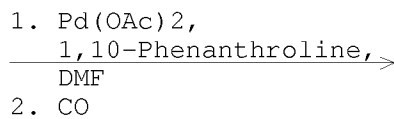
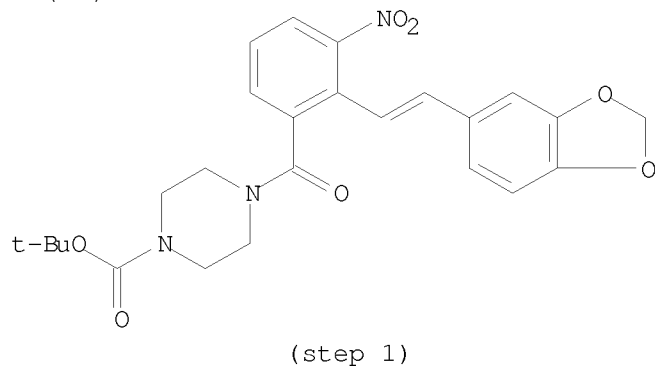


REF: Tetrahedron, 62(49), 11381-11390; 2006

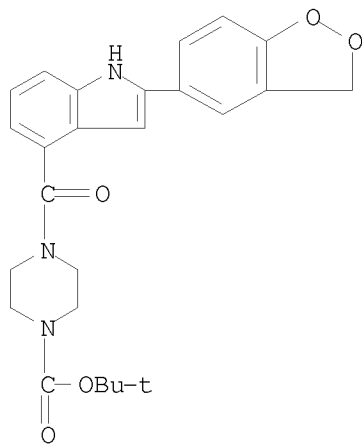
CON: STAGE(1) room temperature -> 80 deg C

STAGE(2) 16 hours, 80 deg C, 30 psi

RX(25) OF 47



RX(25) OF 47



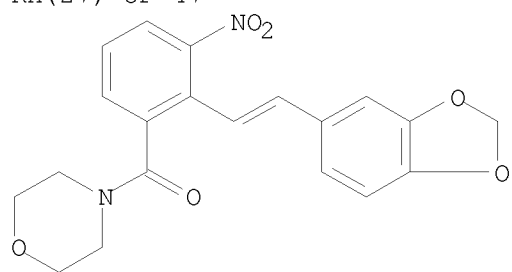
99%

REF: Tetrahedron, 62(49), 11381-11390; 2006

CON: STAGE(1) room temperature -> 80 deg C

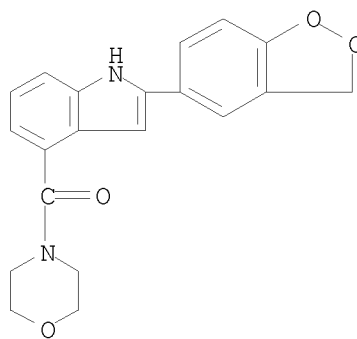
STAGE(2) 16 hours, 80 deg C, 30 psi

RX(27) OF 47



(step 1)

1. Pd(OAc)<sub>2</sub>,  
1,10-Phenanthroline,  
DMF  
2. CO

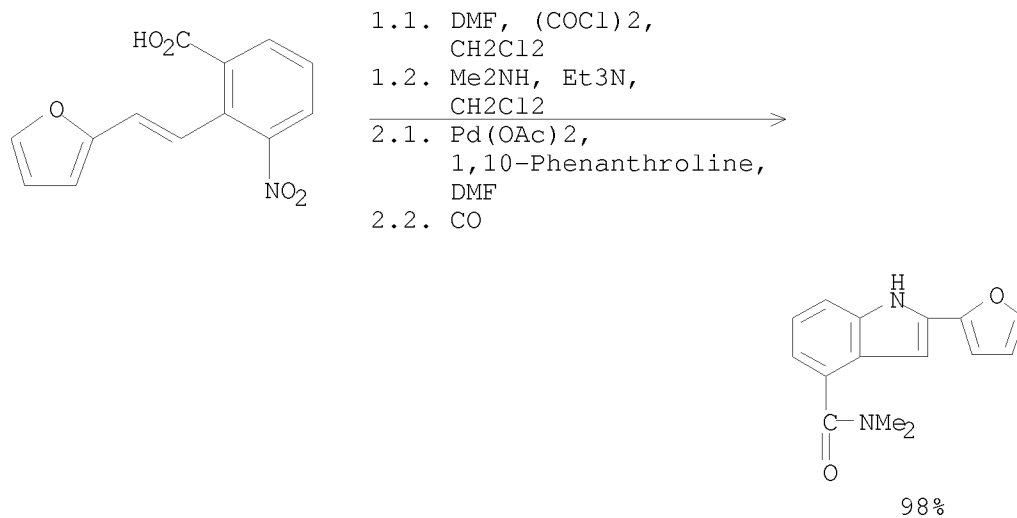


98%

REF: Tetrahedron, 62(49), 11381-11390; 2006

CON: STAGE(1) room temperature -> 80 deg C  
STAGE(2) 16 hours, 80 deg C, 30 psi

RX(37) OF 47 - 2 STEPS

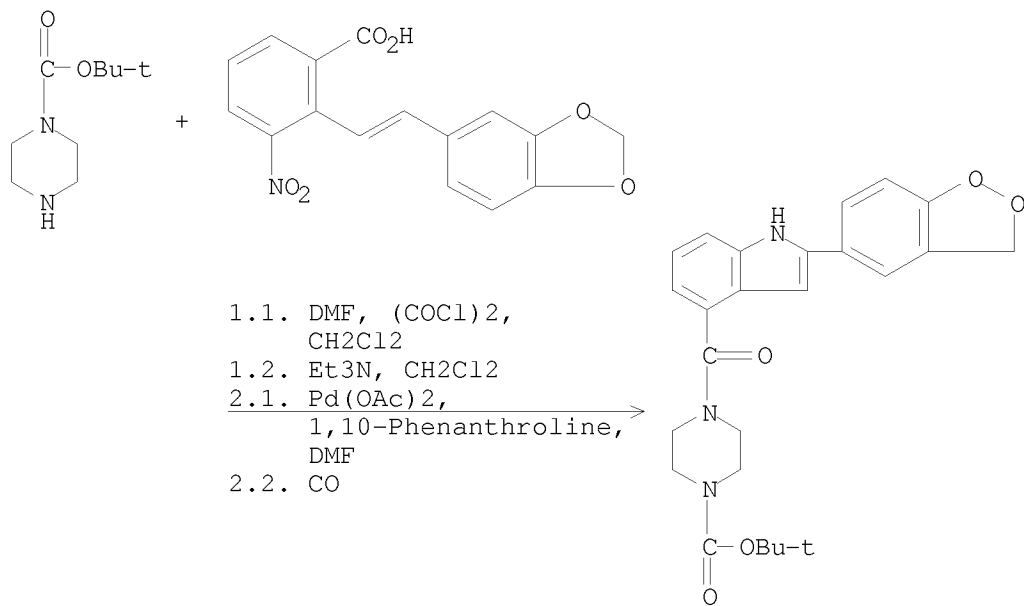


REF: Tetrahedron, 62(49), 11381-11390; 2006

CON: STEP(1.1) 1.5 hours, room temperature  
STEP(1.2) room temperature; 30 minutes, room temperature  
STEP(2.1) room temperature -> 80 deg C  
STEP(2.2) 16 hours, 80 deg C, 30 psi



RX(39) OF 47 - 2 STEPS

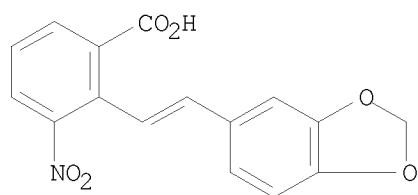


99%

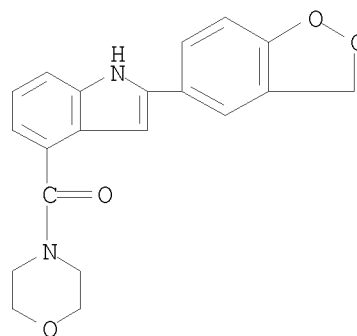
REF: Tetrahedron, 62(49), 11381-11390; 2006

CON: STEP(1.1) 1.5 hours, room temperature  
STEP(1.2) room temperature; 30 minutes, room temperature  
STEP(2.1) room temperature -> 80 deg C  
STEP(2.2) 16 hours, 80 deg C, 30 psi

RX(41) OF 47 - 2 STEPS



- 1.1. DMF, (COCl)<sub>2</sub>,  
CH<sub>2</sub>Cl<sub>2</sub>  
1.2. Morpholine, Et<sub>3</sub>N,  
CH<sub>2</sub>Cl<sub>2</sub>  
2.1. Pd(OAc)<sub>2</sub>,  
1,10-Phenanthroline,  
DMF  
2.2. CO



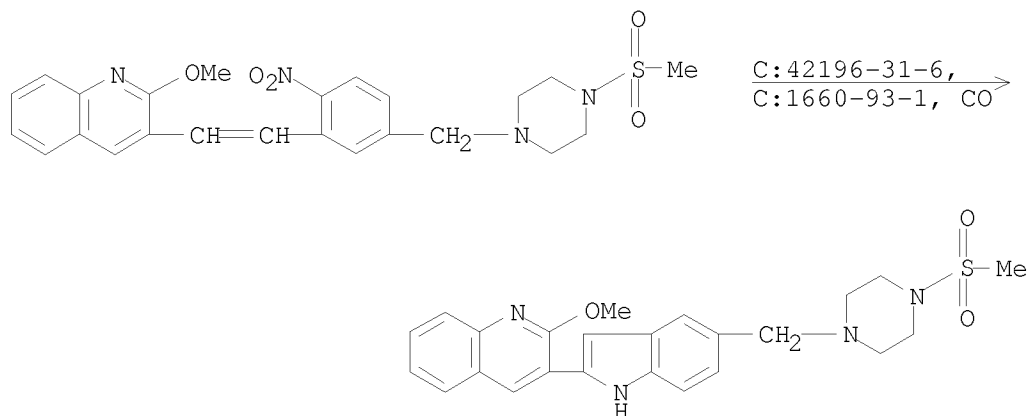
98%

REF: Tetrahedron, 62(49), 11381-11390; 2006

CON: STEP(1.1) 1.5 hours, room temperature  
STEP(1.2) room temperature; 30 minutes, room temperature  
STEP(2.1) room temperature -> 80 deg C  
STEP(2.2) 16 hours, 80 deg C, 30 psi

L4 ANSWER 2 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(2) OF 2



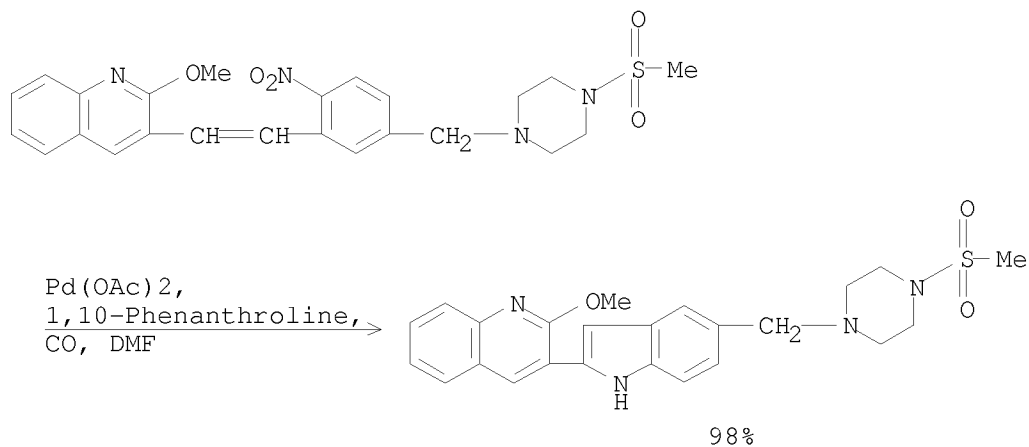
REF: JALA, 10(6), 394-407; 2005

NOTE: optimization study, optimized on catalyst loading, optimized on pressure, optimized on temperature

CON: 70 - 80 deg C, 15 psi

L4 ANSWER 3 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(1) OF 47

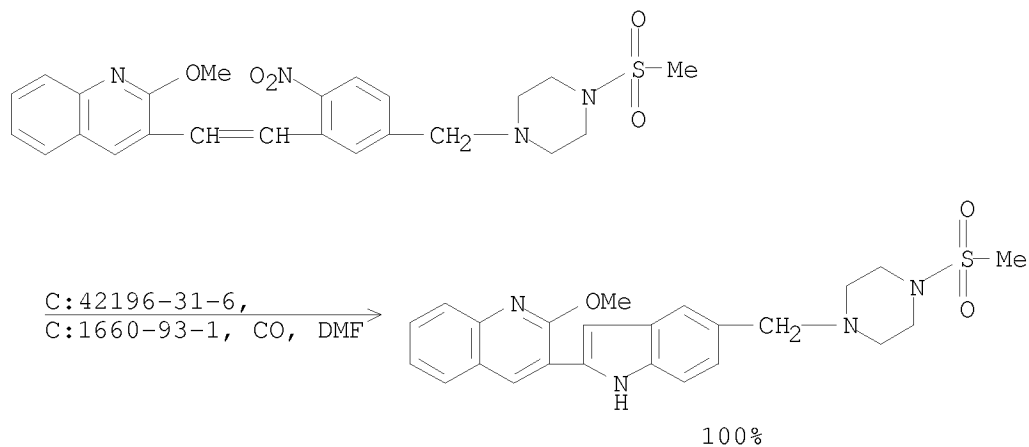


REF: Tetrahedron, 61(26), 6425-6437; 2005

NOTE: optimization study, green chem. - waste reduction

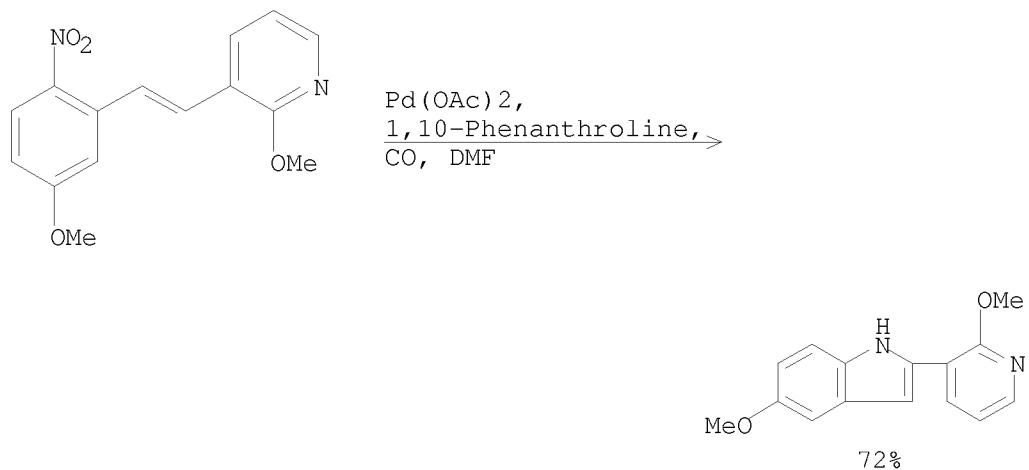
CON: 70 deg C, 15 psi

RX(2) OF 47



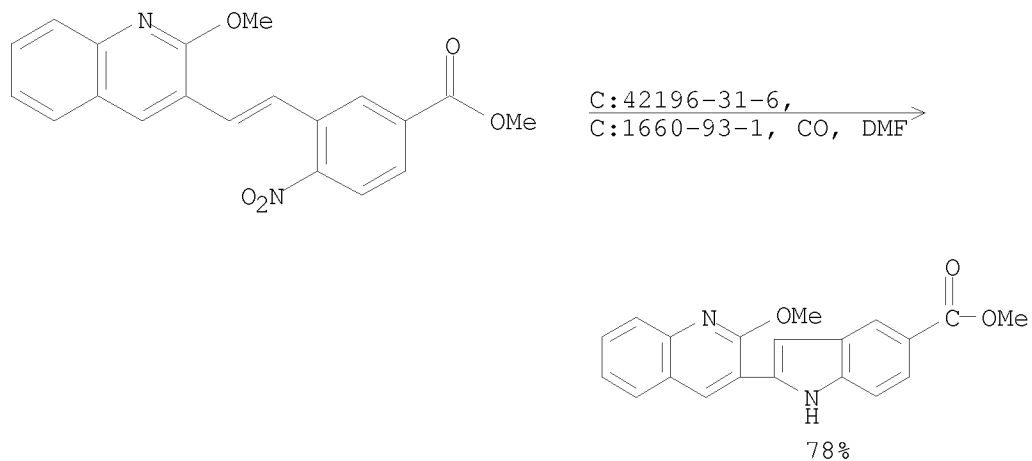
REF: Tetrahedron, 61(26), 6425-6437; 2005  
 NOTE: optimization study, green chem. - waste reduction  
 CON: 70 deg C, 15 psi

RX(23) OF 47



REF: Tetrahedron, 61(26), 6425-6437; 2005  
 NOTE: green chem. - waste reduction  
 CON: 16 hours, 70 deg C, 30 psi

RX(24) OF 47

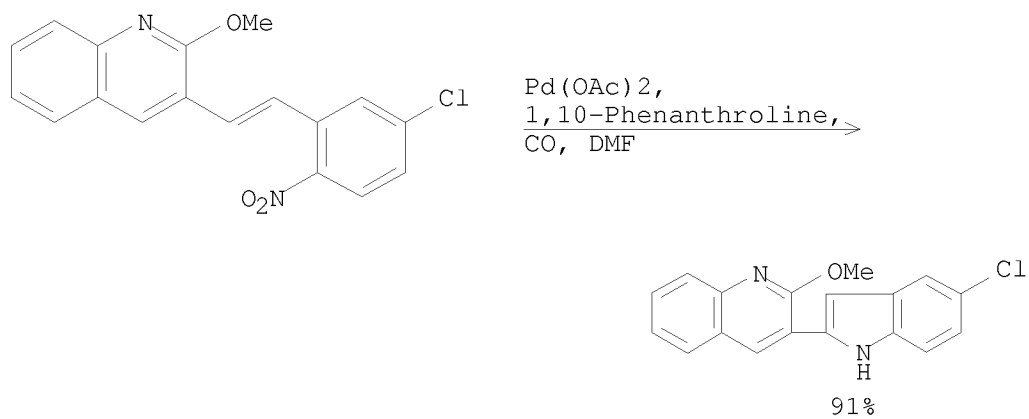


REF: Tetrahedron, 61(26), 6425-6437; 2005

NOTE: green chem. - waste reduction

CON: 16 hours, 80 deg C, 15 psi

RX(25) OF 47

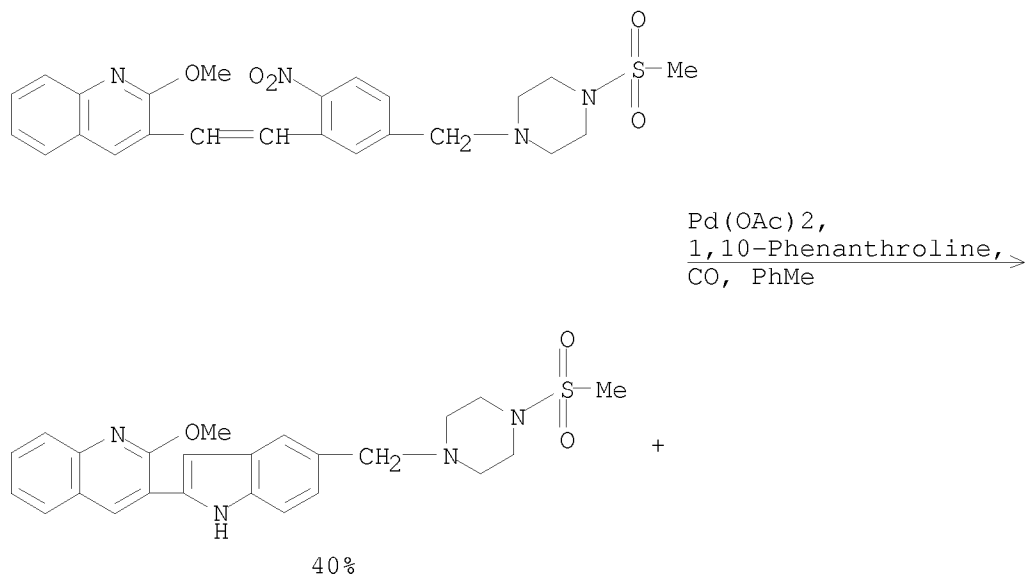


REF: Tetrahedron, 61(26), 6425-6437; 2005

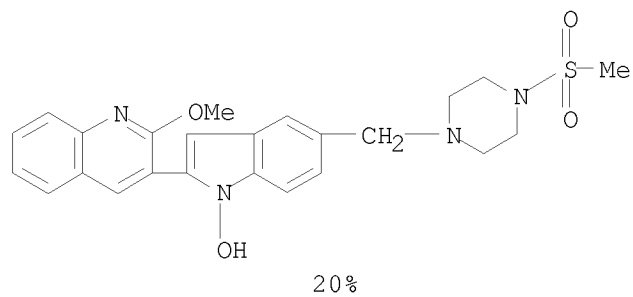
NOTE: green chem. - waste reduction

CON: 16 hours, 80 deg C, 15 psi

RX(28) OF 47

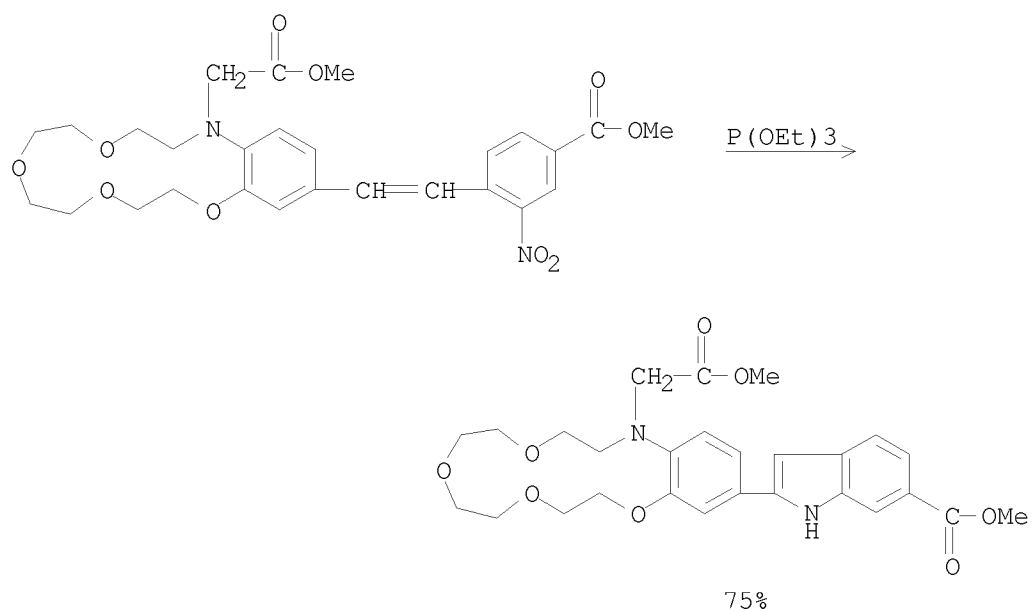


RX(28) OF 47



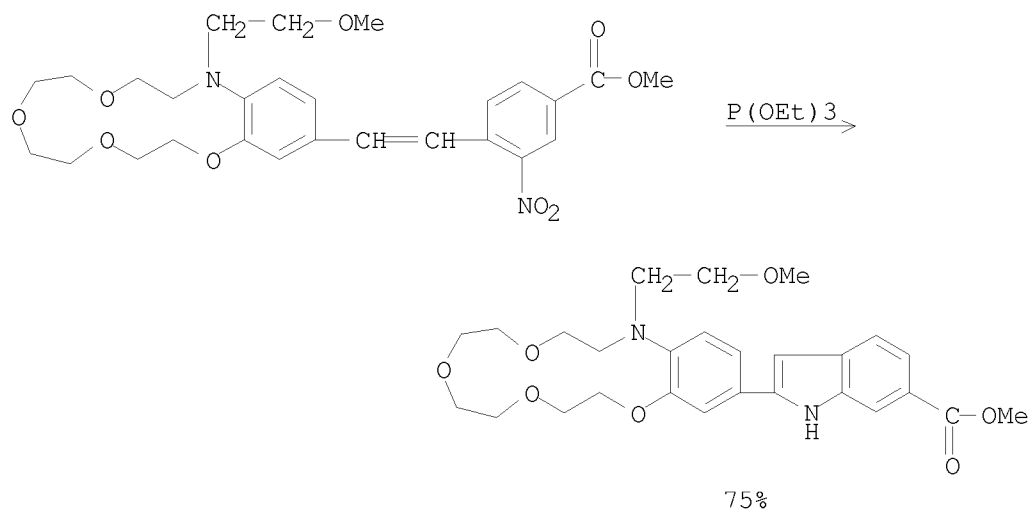
REF: Tetrahedron, 61(26), 6425-6437; 2005  
 CON: 70 deg C, 15 psi

RX(28) OF 161



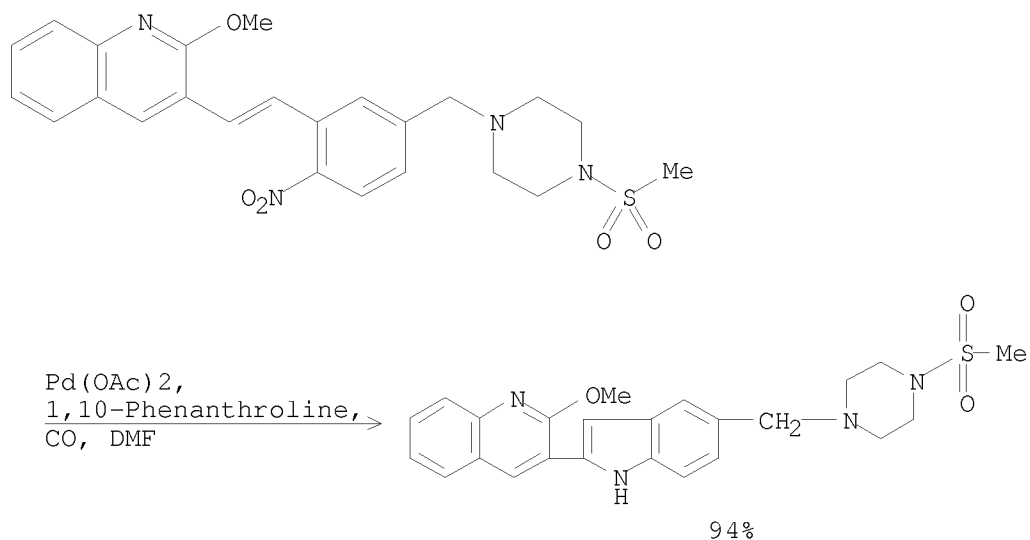
REF: Bioorganic & Medicinal Chemistry Letters, 15(7), 1851-1855; 2005

RX(29) OF 161



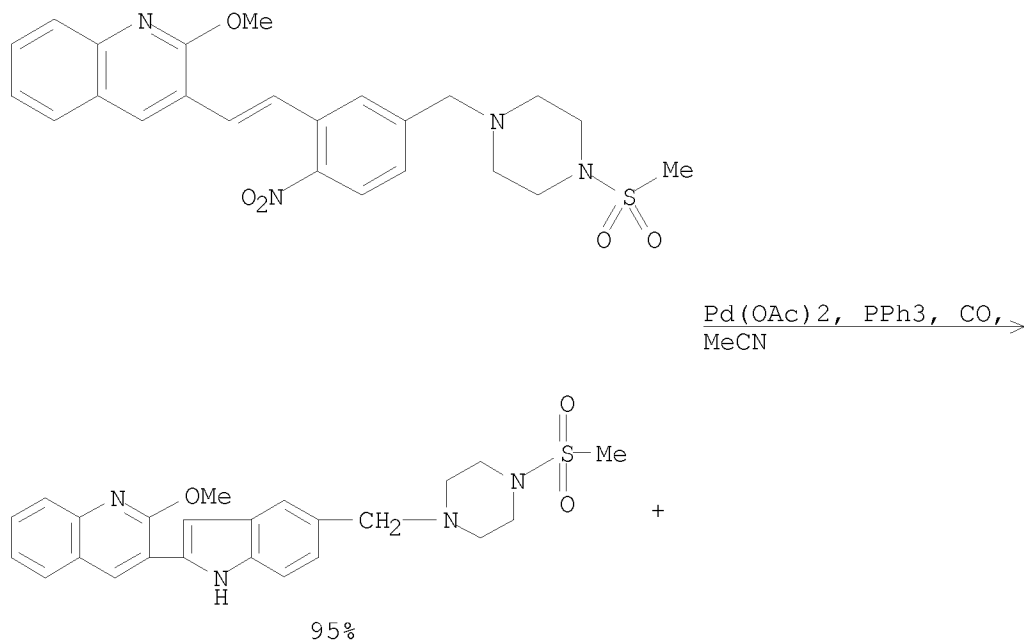
REF: Bioorganic & Medicinal Chemistry Letters, 15(7), 1851-1855; 2005

RX(36) OF 350



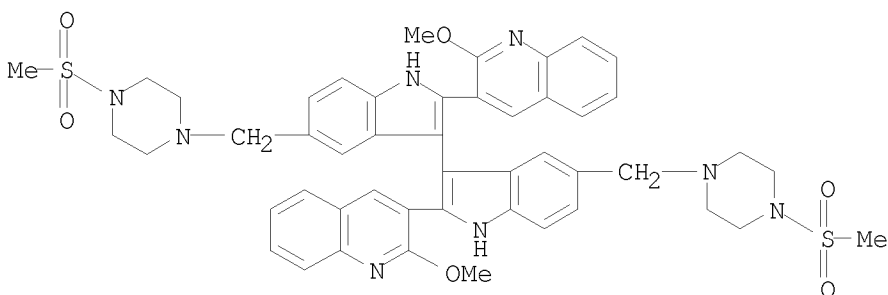
REF: Journal of Organic Chemistry, 70(7), 2555-2567; 2005  
 CON: 14 hours, 70 deg C, 15 psi

RX(37) OF 350



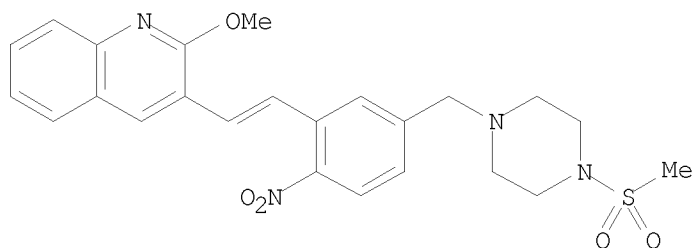


RX(37) OF 350



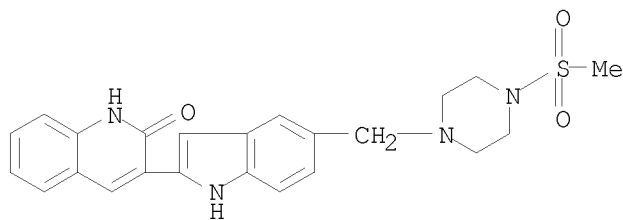
REF: Journal of Organic Chemistry, 70(7), 2555-2567; 2005  
 CON: 15 hours, 70 deg C, 60 atm

RX(59) OF 350 - 2 STEPS



1. Pd(OAc)<sub>2</sub>,  
 1,10-Phenanthroline,  
 CO, DMF  
 2. HCl, Water, DMF

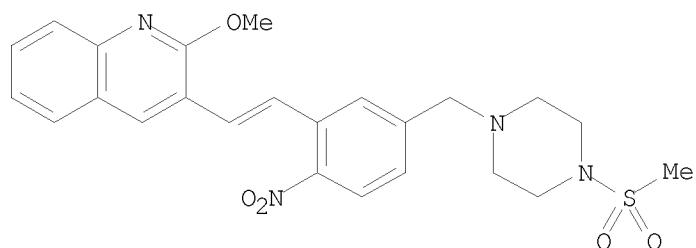
RX(59) OF 350 - 2 STEPS



HCl  
 100%

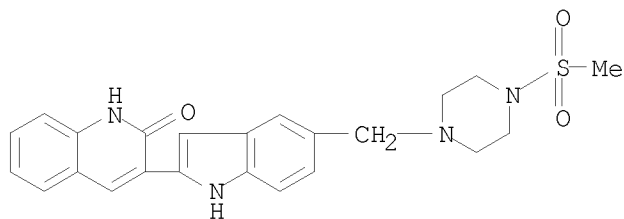
REF: Journal of Organic Chemistry, 70(7), 2555-2567; 2005  
 CON: STEP(1) 14 hours, 70 deg C, 15 psi

RX(60) OF 350 - 2 STEPS



1. Pd(OAc)<sub>2</sub>, PPh<sub>3</sub>, CO,  
MeCN  
2. HCl, Water, DMF →

RX(60) OF 350 - 2 STEPS

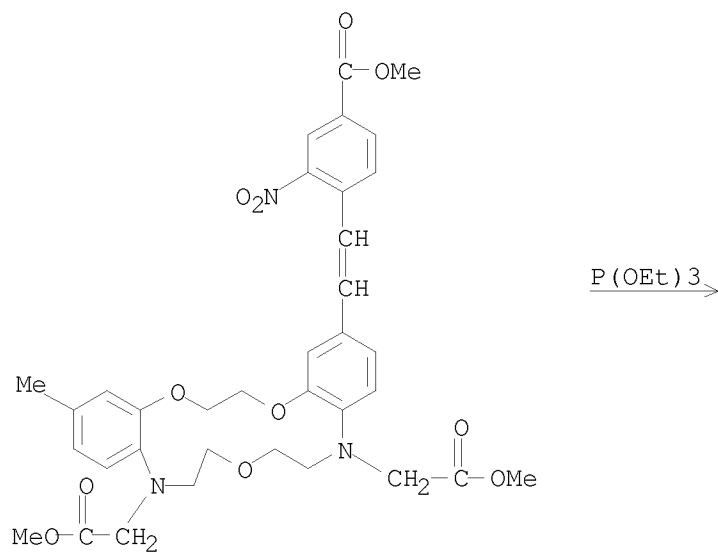


HCl  
100%

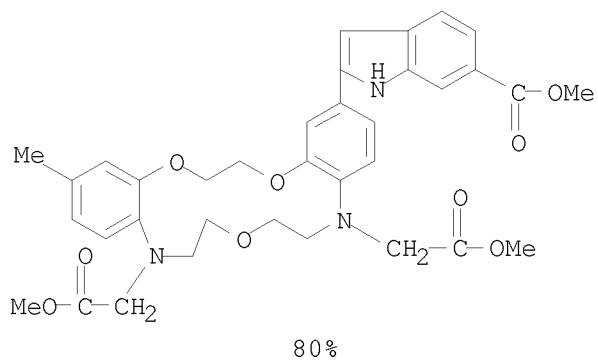
REF: Journal of Organic Chemistry, 70(7), 2555-2567; 2005  
CON: STEP(1) 15 hours, 70 deg C, 60 atm

L4 ANSWER 6 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(26) OF 555



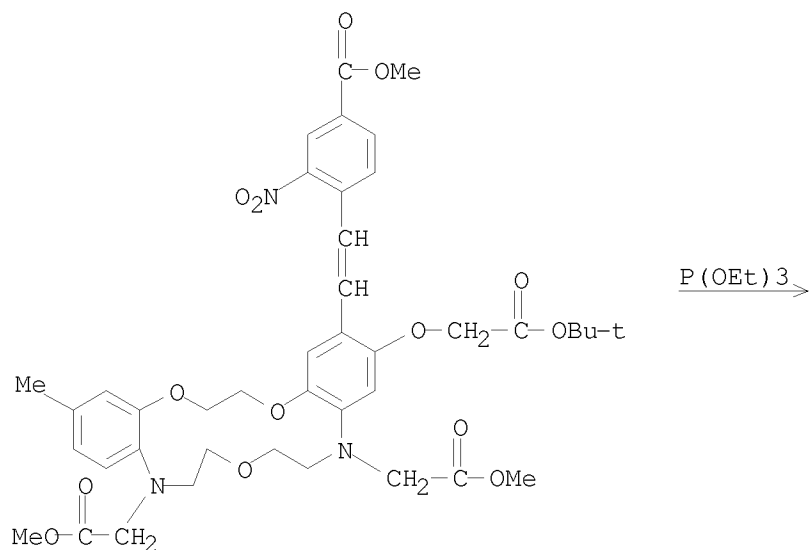
RX(26) OF 555



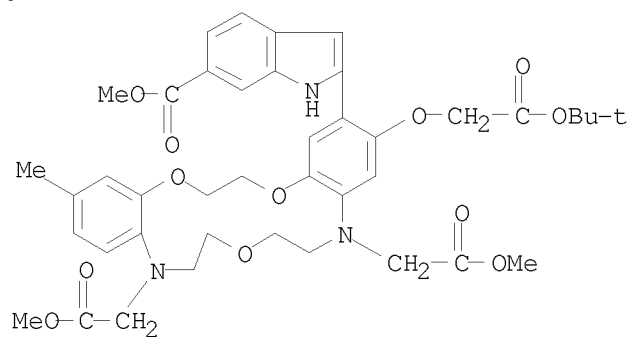
80%

REF: PCT Int. Appl., 2005016874, 24 Feb 2005  
CON: 6 hours, 120 deg C

RX(48) OF 555



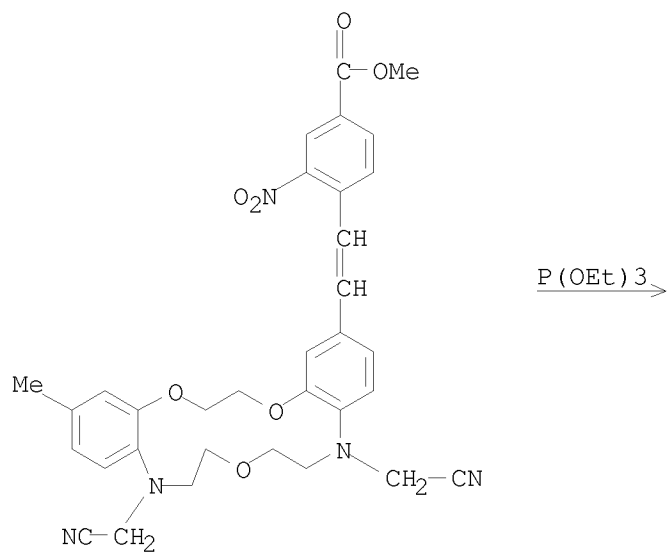
RX(48) OF 555



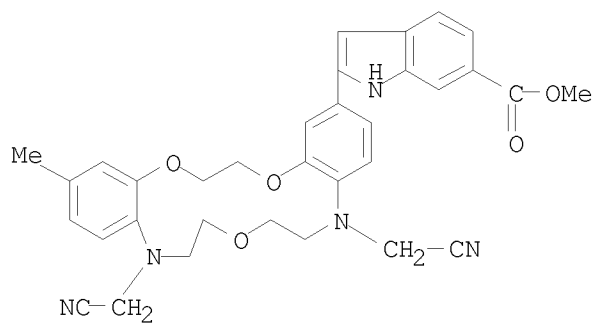
34%

REF: PCT Int. Appl., 136 pp.; 2005  
CON: 7 hours, 130 deg C

RX(54) OF 555



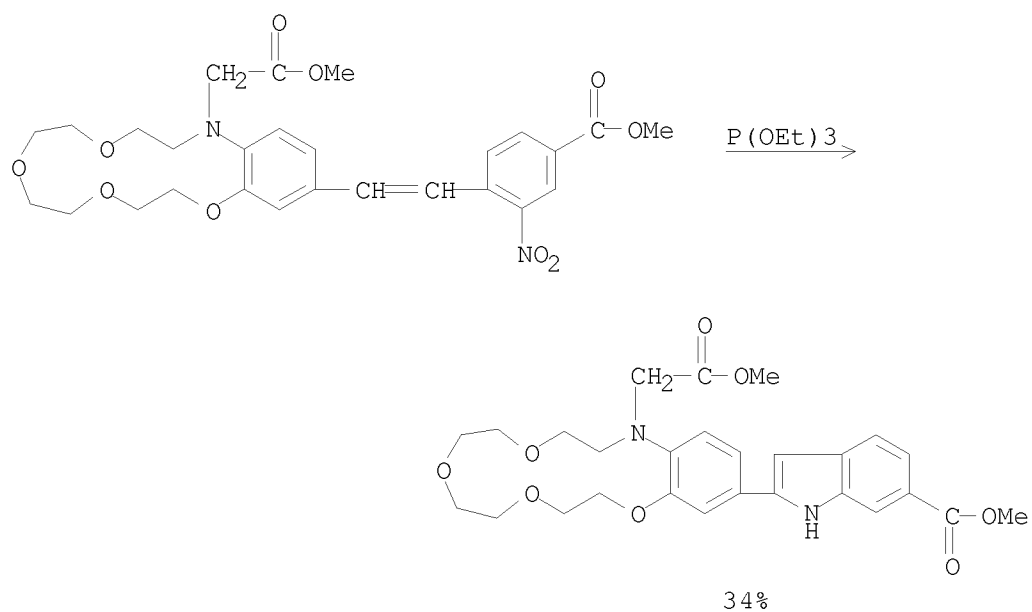
RX(54) OF 555



16%

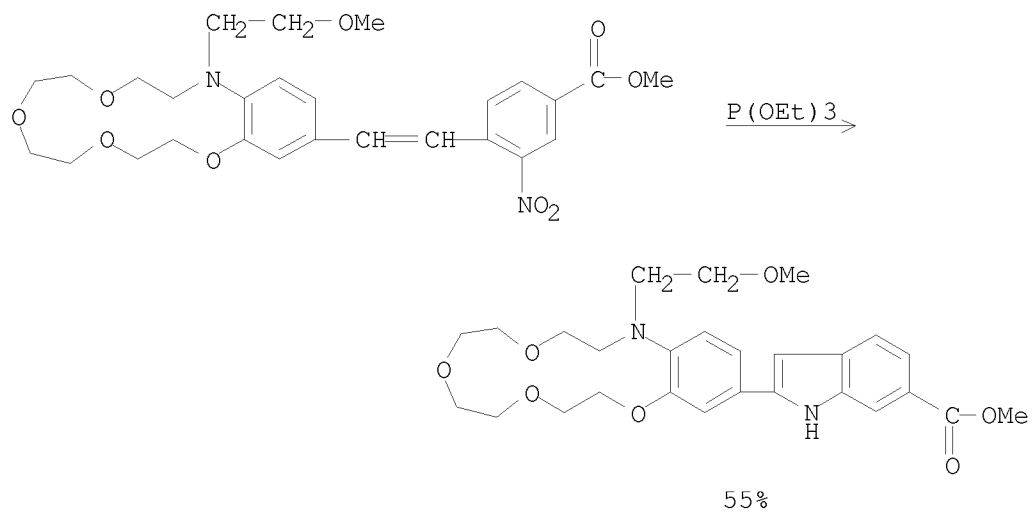
REF: PCT Int. Appl., 136 pp.; 2005  
CON: 16 hours, 120 deg C

RX(67) OF 555



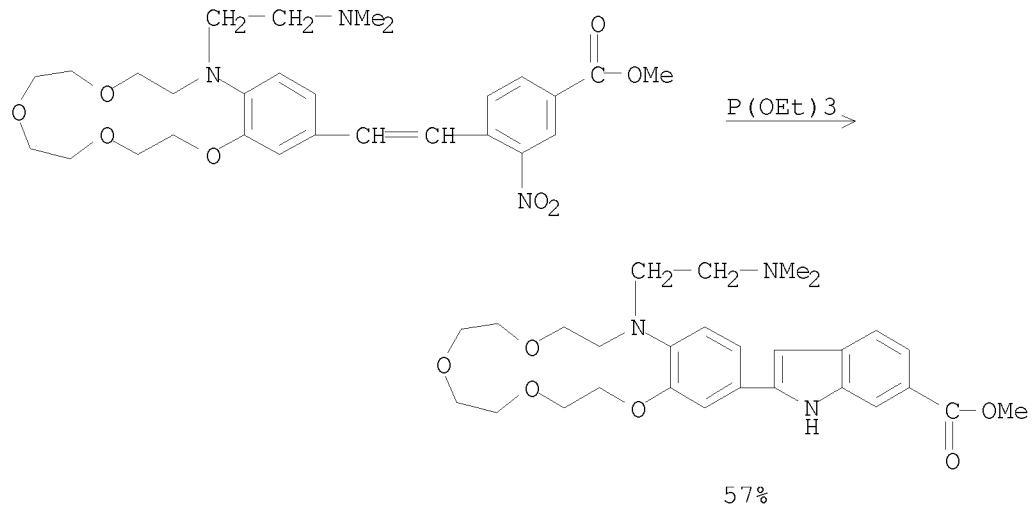
REF: PCT Int. Appl., 136 pp.; 2005  
CON: 4 hours, 125 deg C

RX(91) OF 555



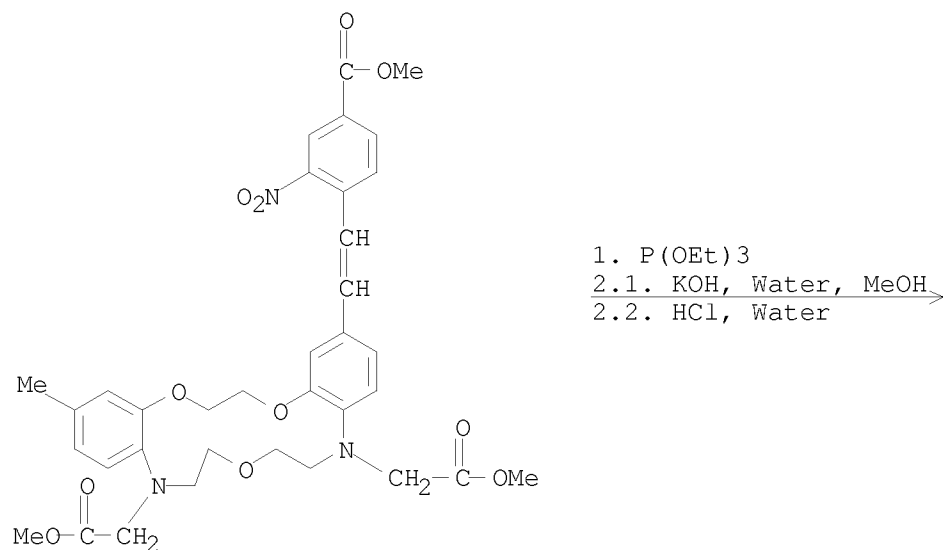
REF: PCT Int. Appl., 136 pp.; 2005  
CON: 4 hours, 125 deg C

RX(97) OF 555

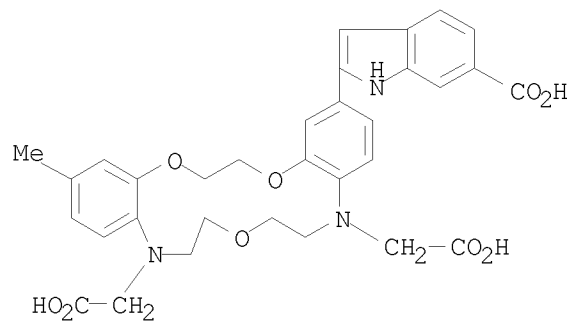


REF: PCT Int. Appl., 136 pp.; 2005  
 CON: 14 hours, 125 deg C

RX(132) OF 555 - 2 STEPS



## RX(132) OF 555 - 2 STEPS



57%

REF: PCT Int. Appl., 136 pp.; 2005

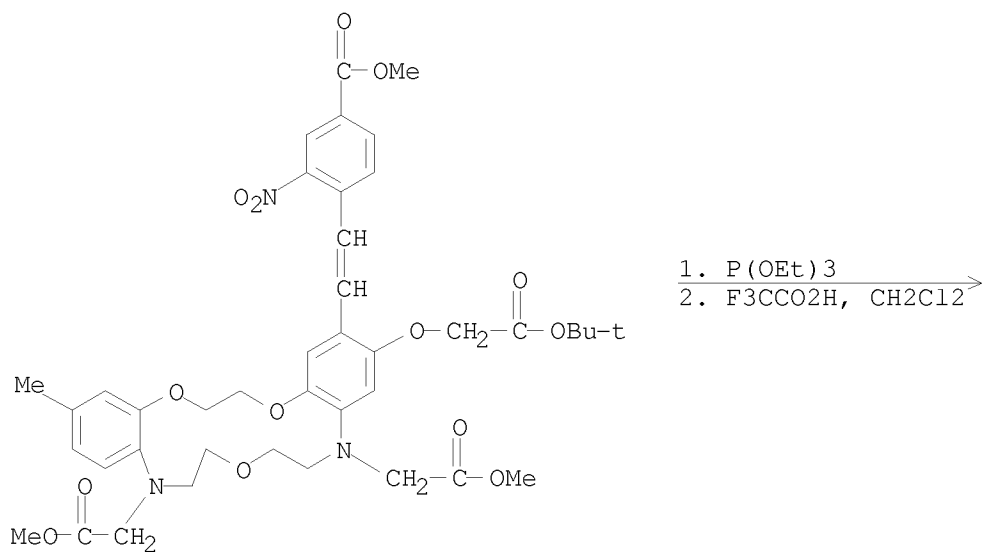
NOTE: 2) incremental addition of reagent in stage 1

CON: STEP(1) 6 hours, 120 deg C

STEP(2.1) 22 hours, room temperature

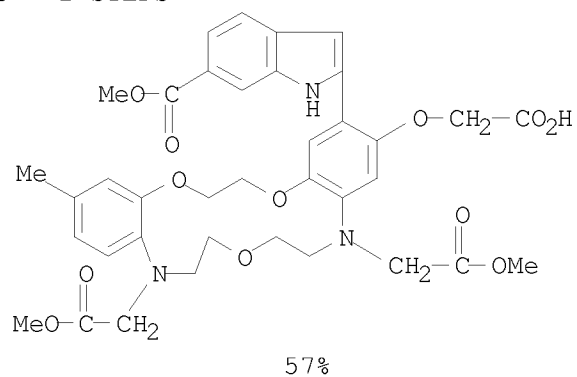
STEP (2.2) room temperature, pH 3

## RX(151) OF 555 - 2 STEPS



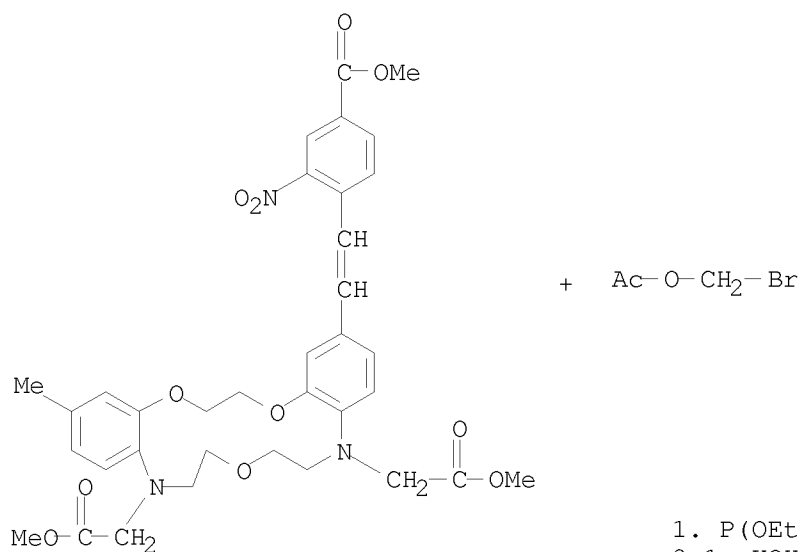


RX(151) OF 555 - 2 STEPS



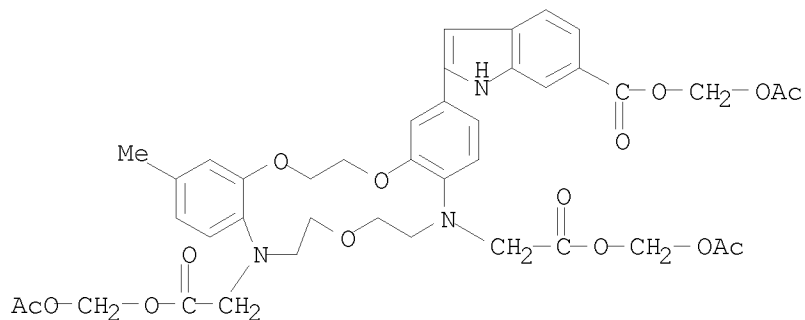
REF: PCT Int. Appl., 136 pp.; 2005  
 CON: STEP(1) 7 hours, 130 deg C  
 STEP(2) 3 hours, room temperature

RX(270) OF 555 - 3 STEPS



1. P(OEt)<sub>3</sub>  
 2.1. KOH, Water, MeOH  
 2.2. HCl, Water  
 3.1. EtN(Pr-i)<sub>2</sub>, DMF  
 3.2. AcOH, Water

RX(270) OF 555 - 3 STEPS



3%

REF: PCT Int. Appl., 136 pp.; 2005

NOTE: 2) incremental addition of reagent in stage 1

CON: STEP(1) 6 hours, 120 deg C

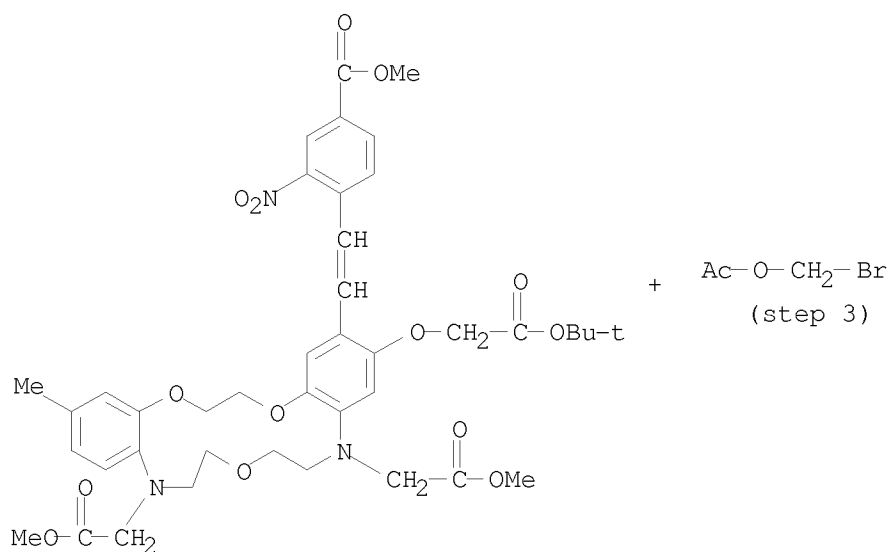
STEP(2.1) 22 hours, room temperature

STEP(2.2) room temperature, pH 3

STEP(3.1) 16 hours, room temperature

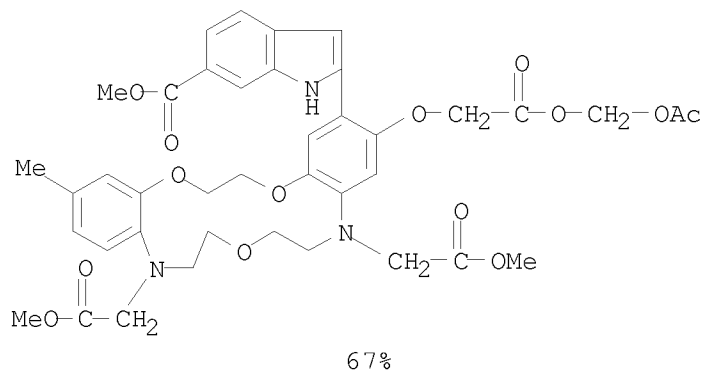
STEP(3.2) room temperature

RX(300) OF 555 - 3 STEPS



1. P(OEt)<sub>3</sub>
2. F<sub>3</sub>CCO<sub>2</sub>H, CH<sub>2</sub>Cl<sub>2</sub>
3. EtN(Pr-i)<sub>2</sub>, DMF

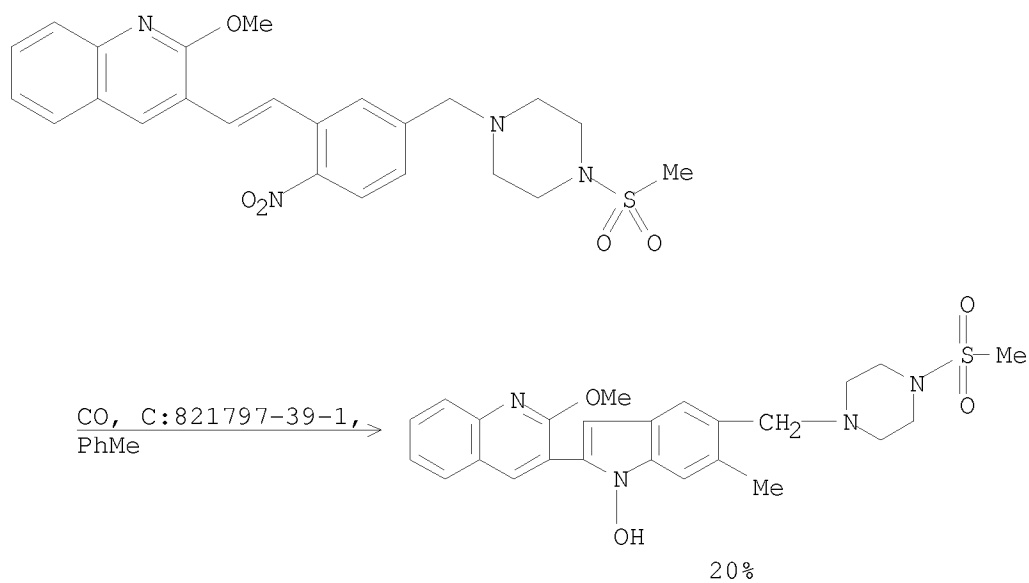
RX(300) OF 555 - 3 STEPS



REF: PCT Int. Appl., 136 pp.; 2005  
 CON: STEP(1) 7 hours, 130 deg C  
 STEP(2) 3 hours, room temperature  
 STEP(3) 16 hours, room temperature

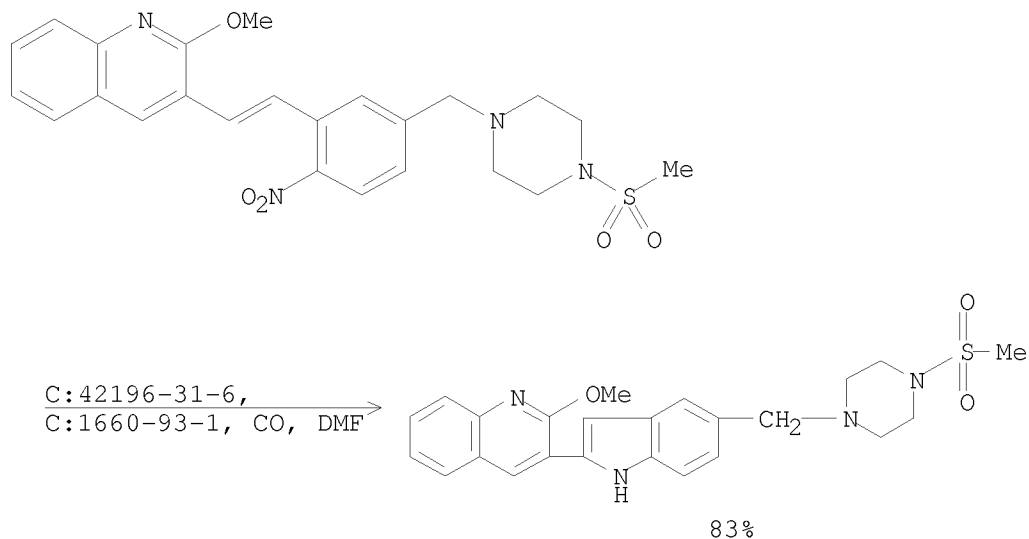
L4 ANSWER 7 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(5) OF 30



REF: PCT Int. Appl., 2005000804, 06 Jan 2005  
 NOTE: Endeavor reactor was used  
 CON: STAGE(1) room temperature, 15 psi; 16 hours, 70 deg C

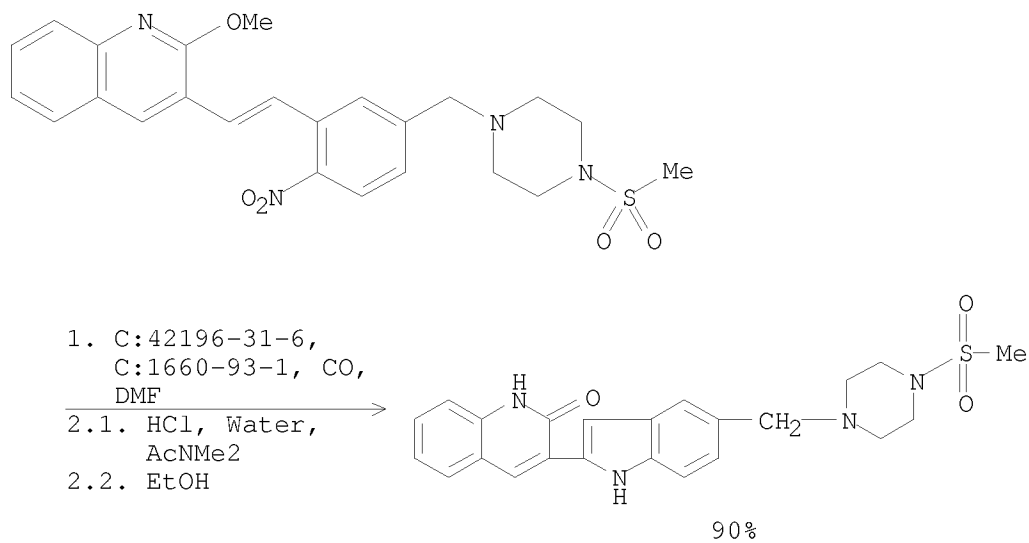
RX(6) OF 30



REF: PCT Int. Appl., 31 pp.; 2005

CON: STAGE(1) room temperature, 15 psi; 14 hours, 70 deg C

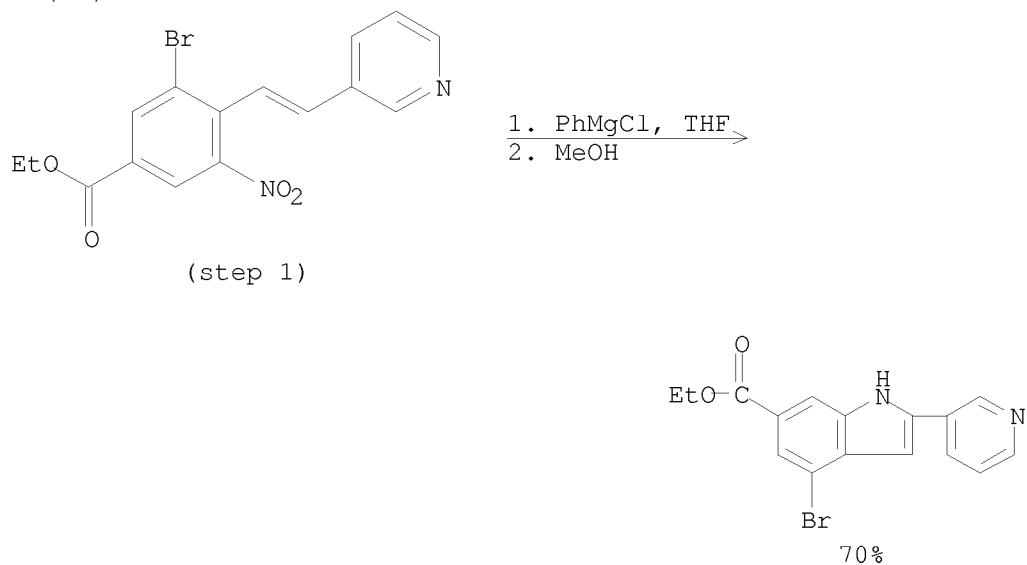
RX(13) OF 30 - 2 STEPS



REF: PCT Int. Appl., 31 pp.; 2005

CON: STEP(1.1) room temperature, 15 psi; 14 hours, 70 deg C  
STEP(2.1) 2 hours; 60 deg C

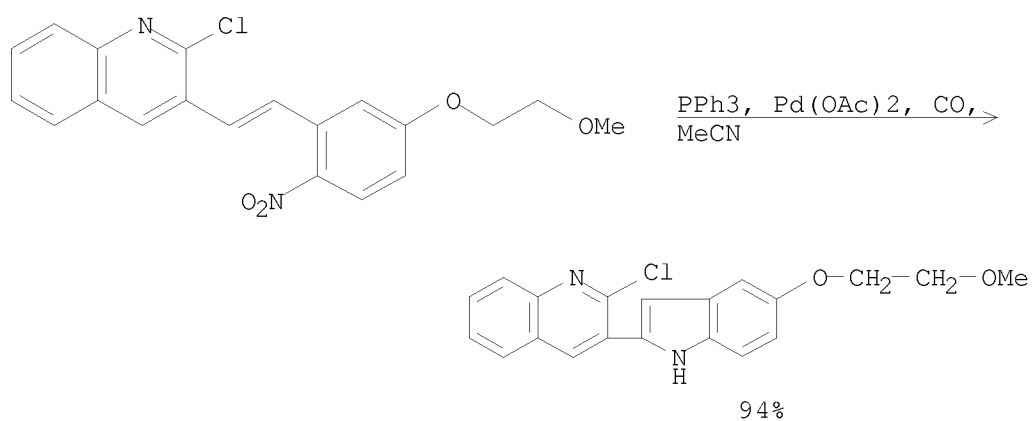
RX(37) OF 85



REF: Chemistry--A European Journal, 9(21), 5323-5331; 2003  
 CON: 30 minutes, -40 deg C

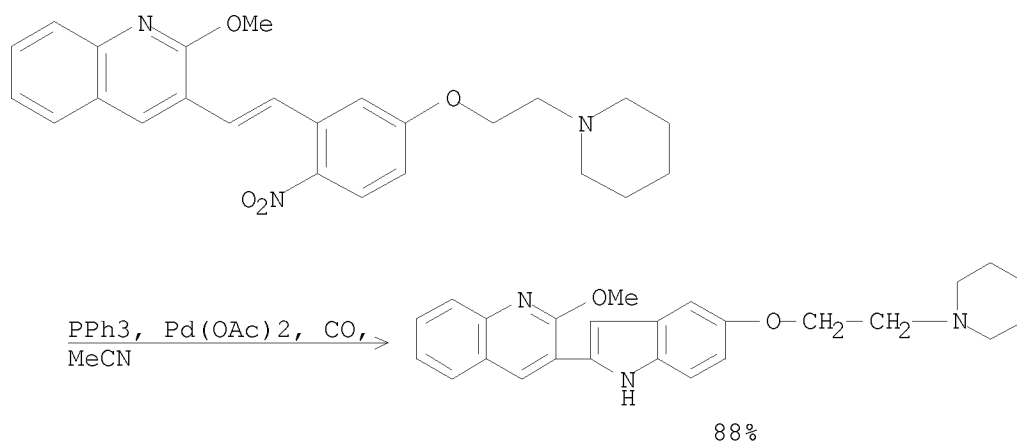
L4 ANSWER 9 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(4) OF 63



REF: Organic Letters, 5(21), 3975-3978; 2003  
 NOTE: alternative prepn. shown  
 CON: 12 hours, 70 deg C, 6 atm

RX(10) OF 63

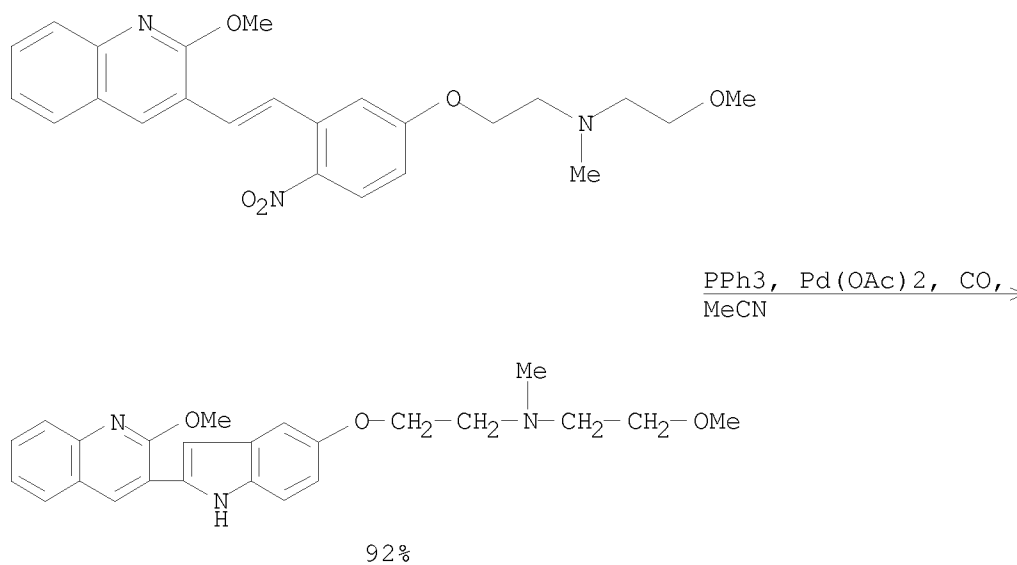


REF: Organic Letters, 5(21), 3975-3978; 2003

NOTE: alternative prepn. shown

CON: 12 hours, 70 deg C, 6 atm

RX(15) OF 63

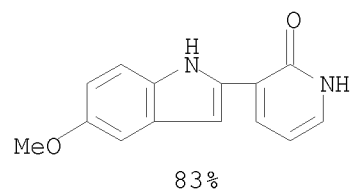
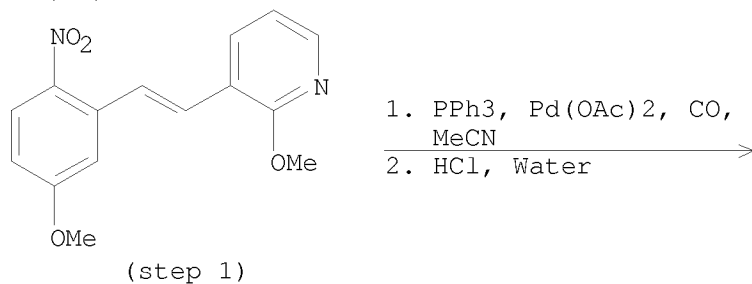


REF: Organic Letters, 5(21), 3975-3978; 2003

NOTE: alternative prepn. shown

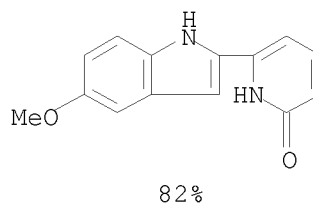
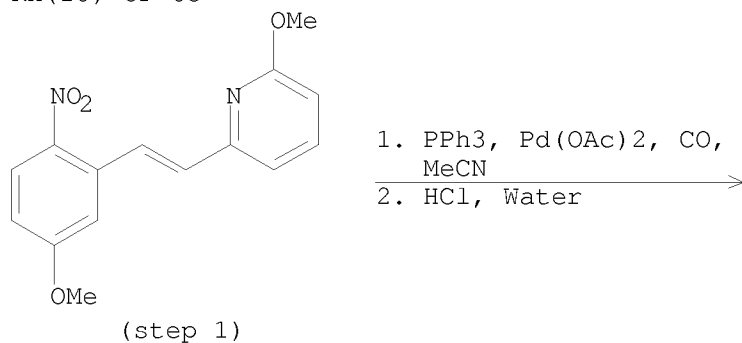
CON: 12 hours, 70 deg C, 6 atm

RX(17) OF 63



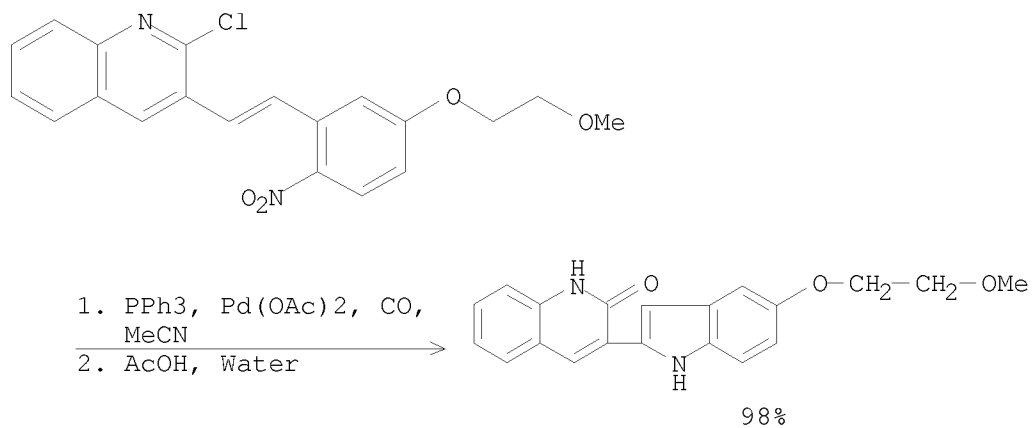
REF: Organic Letters, 5(21), 3975-3978; 2003  
CON: STAGE(1) 12 hours, 70 deg C, 6 atm  
STAGE(2) 12 hours, reflux

RX(18) OF 63



REF: Organic Letters, 5(21), 3975-3978; 2003  
CON: STAGE(1) 12 hours, 70 deg C, 6 atm  
STAGE(2) 12 hours, reflux

RX(25) OF 63 - 2 STEPS



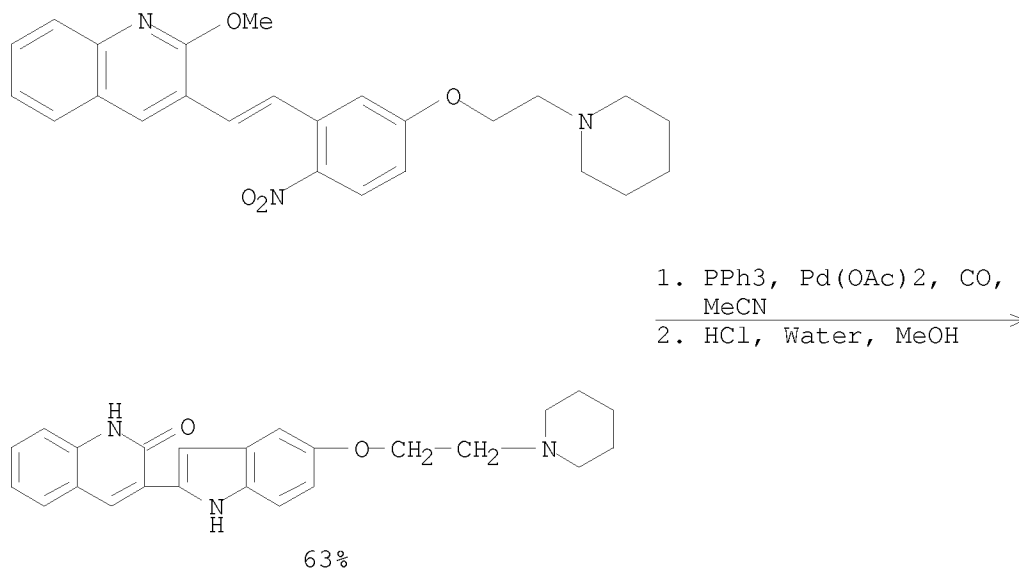
REF: Organic Letters, 5(21), 3975-3978; 2003

NOTE: 1) alternative prepn. shown, 2) alternative prepn. shown

CON: STEP(1) 12 hours, 70 deg C, 6 atm

STEP(2) 3 hours, reflux

RX(29) OF 63 - 2 STEPS



REF: Organic Letters, 5(21), 3975-3978; 2003

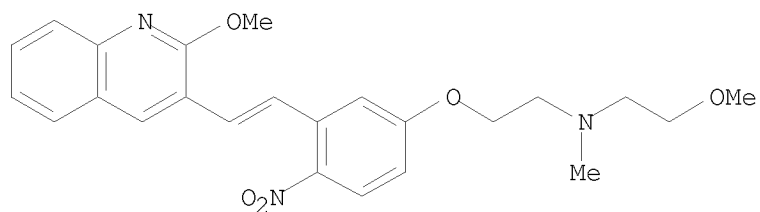
NOTE: 1) alternative prepn. shown

CON: STEP(1) 12 hours, 70 deg C, 6 atm

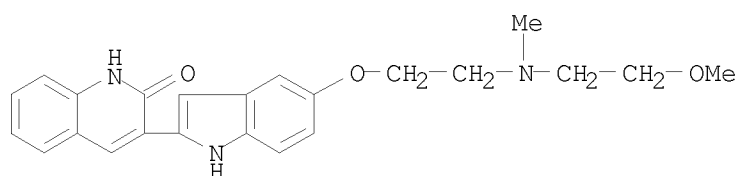
STEP(2) 4 hours, reflux



RX(33) OF 63 - 2 STEPS



1. PPh<sub>3</sub>, Pd(OAc)<sub>2</sub>, CO,  
MeCN  
2. HCl, Water, MeOH →



REF: Organic Letters, 5(21), 3975-3978; 2003

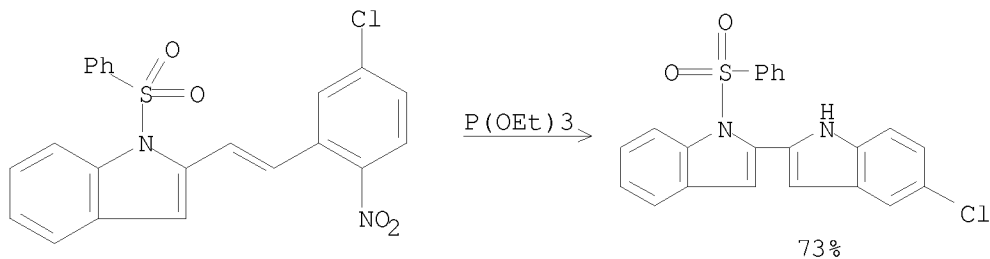
NOTE: 1) alternative prepn. shown

CON: STEP(1) 12 hours, 70 deg C, 6 atm

STEP(2) 4 hours, reflux

L4 ANSWER 10 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

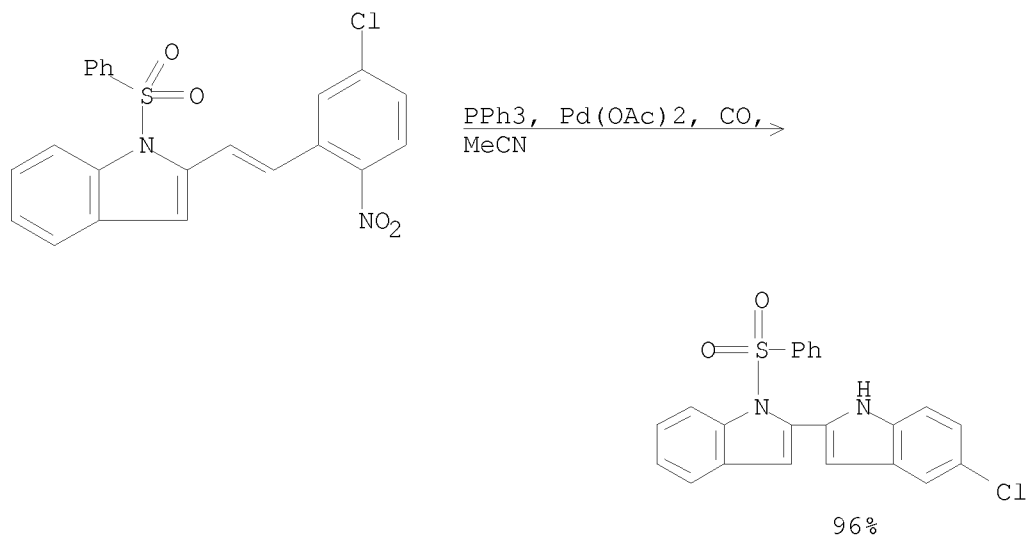
RX(3) OF 71



REF: Organic Letters, 5(20), 3721-3723; 2003

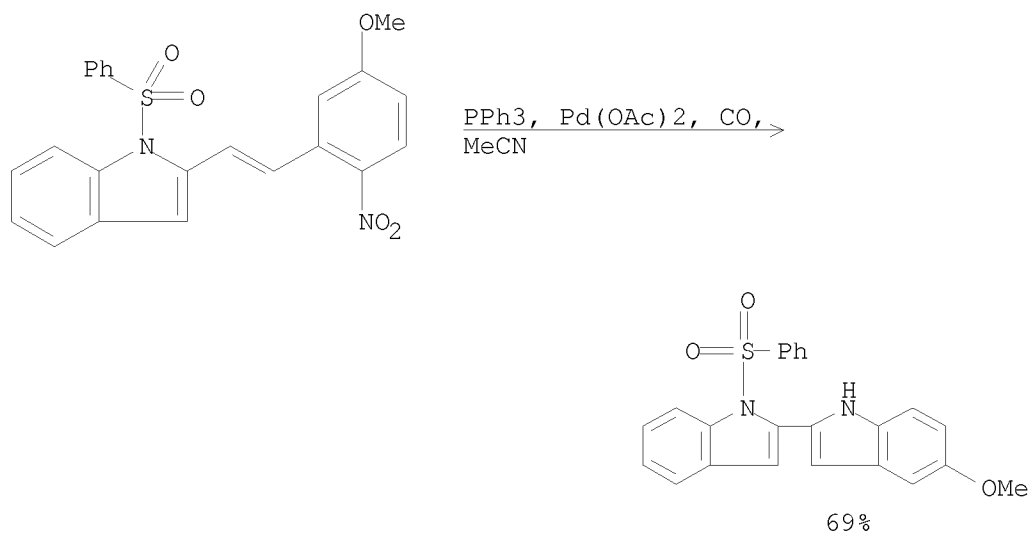
CON: 2 hours, 155 deg C

RX(4) OF 71



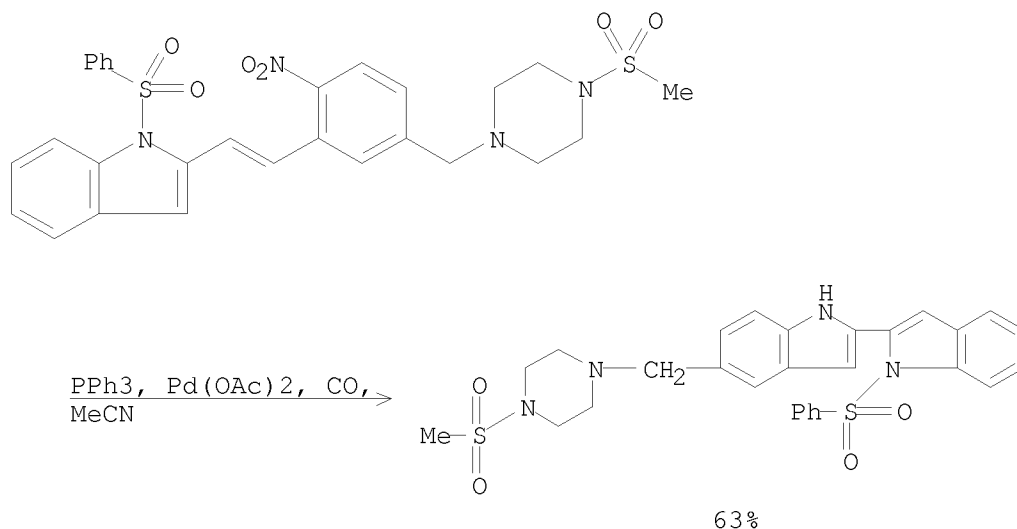
REF: Organic Letters, 5(20), 3721-3723; 2003  
 CON: 12 hours, 70 deg C

RX(6) OF 71



REF: Organic Letters, 5(20), 3721-3723; 2003  
 NOTE: using other method also got good yield  
 CON: 12 hours, 70 deg C

RX(7) OF 71

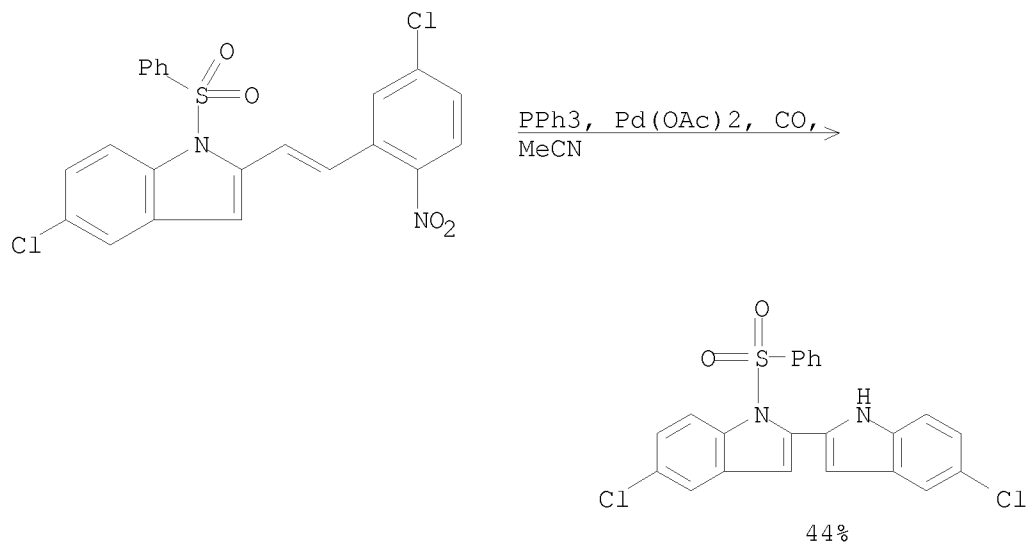


REF: Organic Letters, 5(20), 3721-3723; 2003

NOTE: using other method also got good yield

CON: 12 hours, 70 deg C

RX(9) OF 71

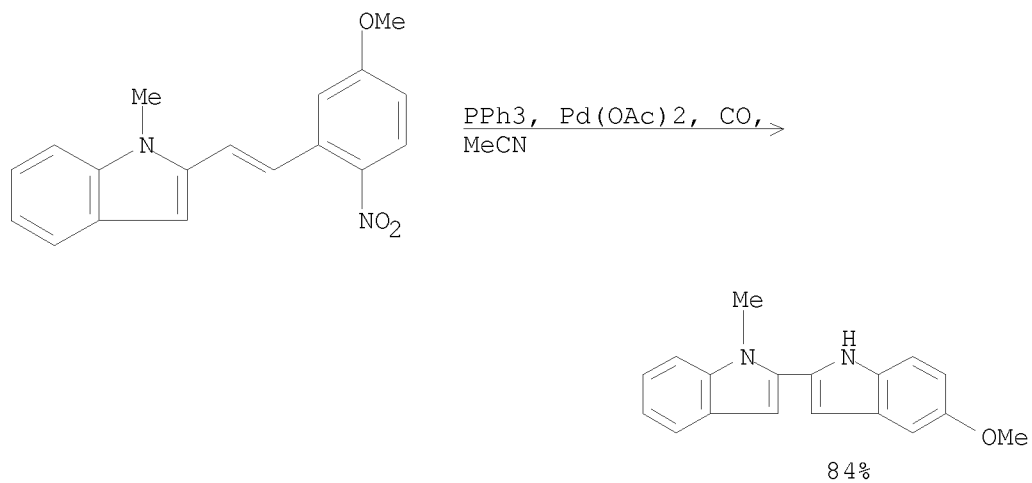


REF: Organic Letters, 5(20), 3721-3723; 2003

NOTE: using other method also got good yield

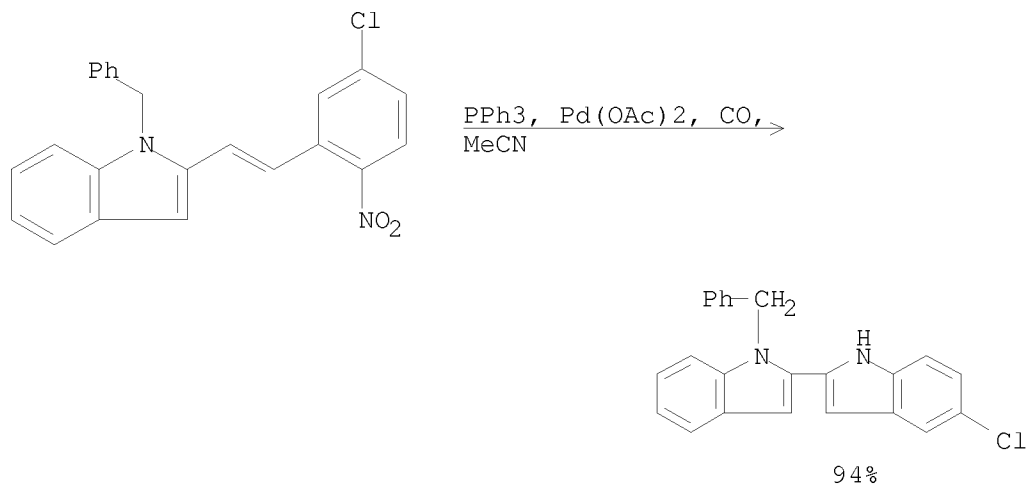
CON: 12 hours, 70 deg C

RX(11) OF 71



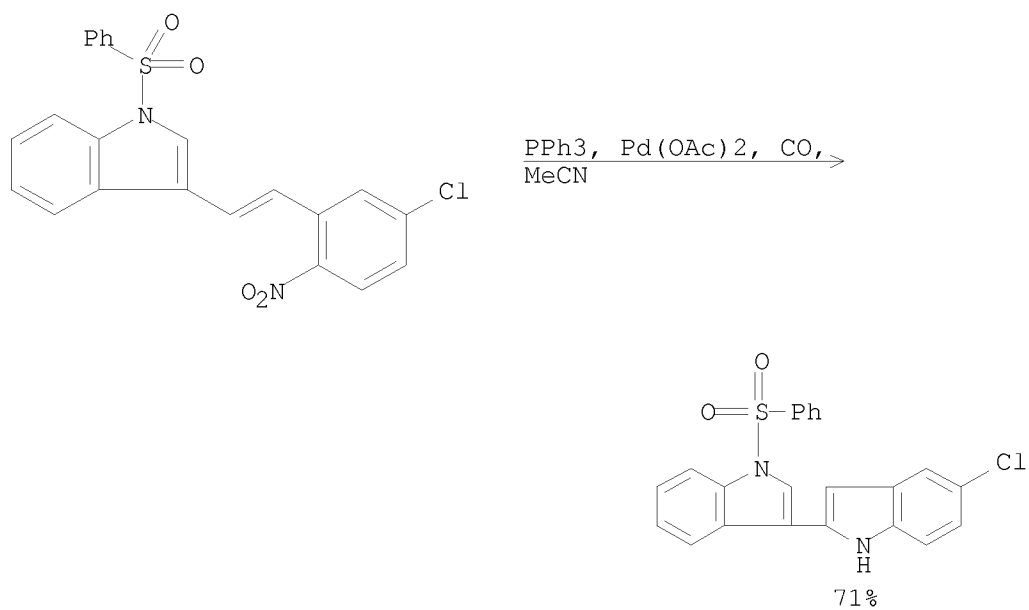
REF: Organic Letters, 5(20), 3721-3723; 2003  
 NOTE: using other method also got good yield  
 CON: 12 hours, 70 deg C

RX(14) OF 71



REF: Organic Letters, 5(20), 3721-3723; 2003  
 NOTE: using other method also got good yield  
 CON: 12 hours, 70 deg C

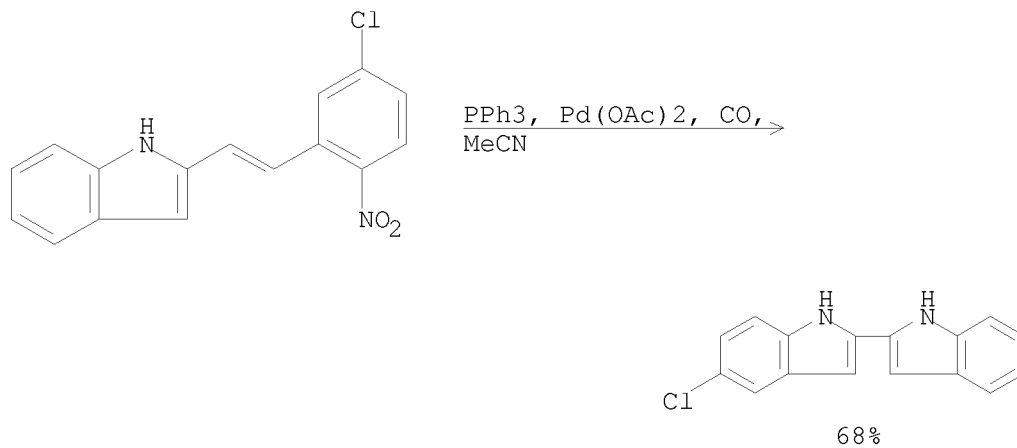
RX(16) OF 71



REF: Organic Letters, 5(20), 3721-3723; 2003

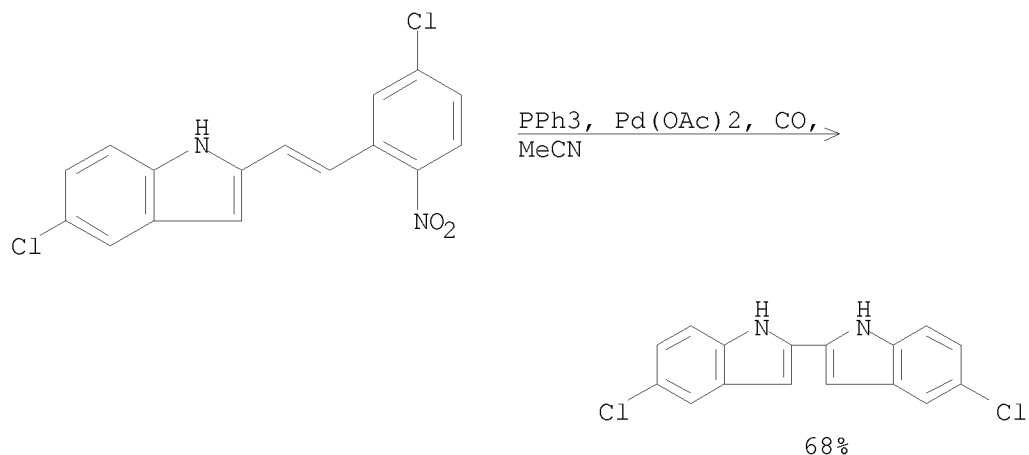
NOTE: using other method also got good yield  
 CON: 12 hours, 70 deg C

RX(18) OF 71



REF: Organic Letters, 5(20), 3721-3723; 2003  
 NOTE: using other method also got good yield  
 CON: 12 hours, 70 deg C

RX(21) OF 71



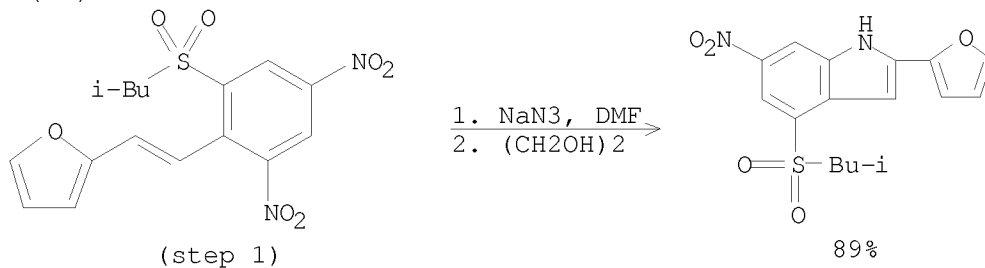
REF: Organic Letters, 5(20), 3721-3723; 2003

NOTE: using other method also got good yield

CON: 12 hours, 70 deg C

L4 ANSWER 11 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(11) OF 29

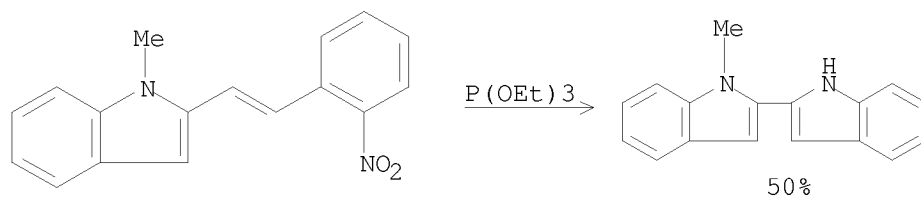


REF: Synthetic Communications, 32(9), 1465-1474; 2002

NOTE: regioselective, thermal, stereoselective

L4 ANSWER 12 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

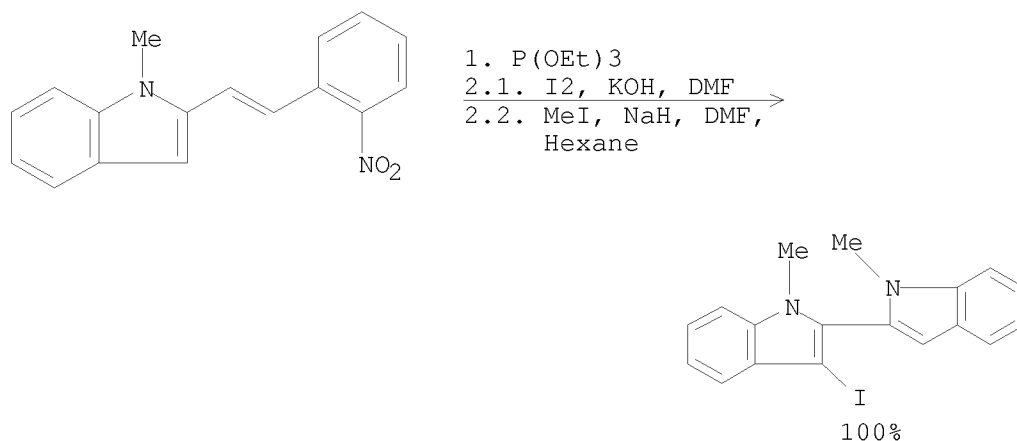
RX(10) OF 177



REF: Tetrahedron, 57(24), 5199-5212; 2001

NOTE: thermal, alternative preps. gave similar yields

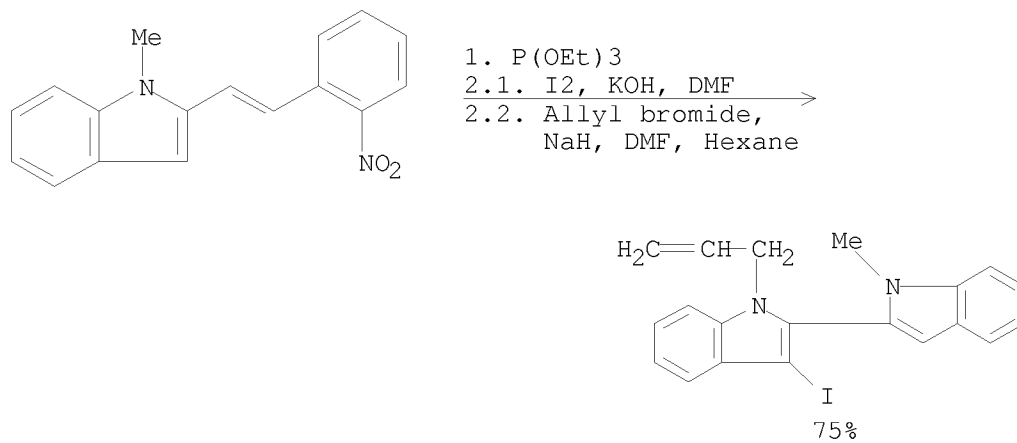
RX(43) OF 177 - 2 STEPS



REF: Tetrahedron, 57(24), 5199-5212; 2001

NOTE: 1) thermal, alternative preps. gave similar yields

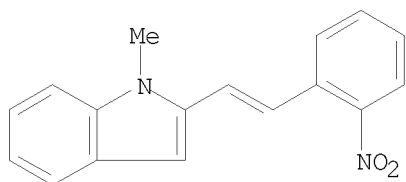
RX(44) OF 177 - 2 STEPS



REF: Tetrahedron, 57(24), 5199-5212; 2001

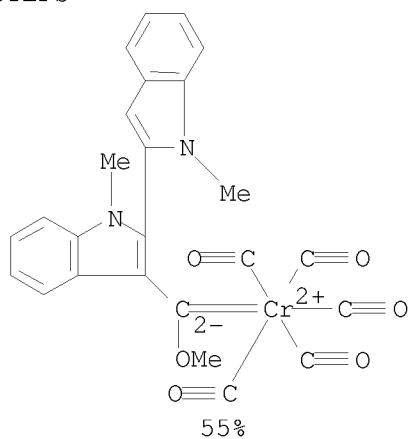
NOTE: 1) thermal, alternative preps. gave similar yields, 2) reactant assumed

RX(79) OF 177 - 3 STEPS



1.  $\text{P}(\text{OEt})_3$
- 2.1.  $\text{I}_2$ ,  $\text{KOH}$ ,  $\text{DMF}$
- 2.2.  $\text{MeI}$ ,  $\text{NaH}$ ,  $\text{DMF}$ ,  
Hexane
- 3.1.  $\text{BuLi}$ ,  $\text{THF}$ ,  $\text{Et}_2\text{O}$
- 3.2.  $\text{Cr}(\text{CO})_6$ ,  $\text{Et}_2\text{O}$
- 3.3.  $\text{Na}_2\text{CO}_3$ , Water
- 3.4.  $\text{CF}_3\text{SO}_3\text{Me}$

RX(79) OF 177 - 3 STEPS

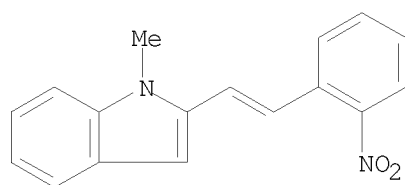


REF: Tetrahedron, 57(24), 5199-5212; 2001

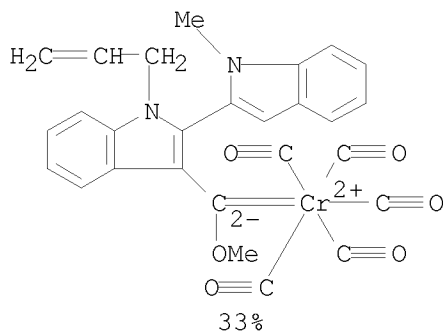
NOTE: 1) thermal, alternative preps. gave similar yields



RX(80) OF 177 - 3 STEPS



1.  $\text{P}(\text{OEt})_3$
- 2.1.  $\text{I}_2$ ,  $\text{KOH}$ ,  $\text{DMF}$
- 2.2. Allyl bromide,  
 $\text{NaH}$ ,  $\text{DMF}$ ,  $\text{Hexane}$
- 3.1.  $\text{BuLi}$ ,  $\text{THF}$ ,  $\text{Et}_2\text{O}$
- 3.2.  $\text{Cr}(\text{CO})_6$ ,  $\text{Et}_2\text{O}$
- 3.3.  $\text{Na}_2\text{CO}_3$ ,  $\text{Water}$
- 3.4.  $\text{CF}_3\text{SO}_3\text{Me}$

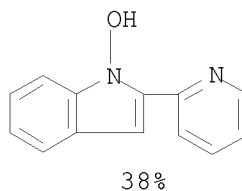
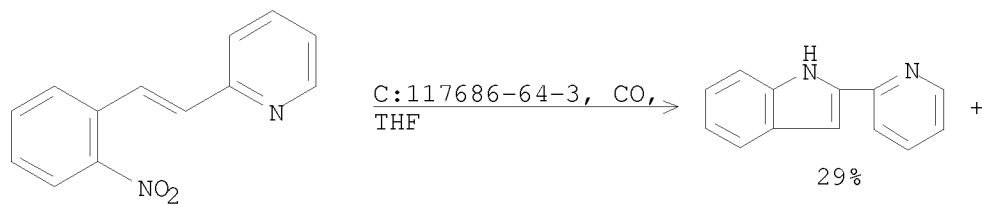


REF: Tetrahedron, 57(24), 5199-5212; 2001

NOTE: 1) thermal, alternative preps. gave similar yields, 2) reactant assumed

L4 ANSWER 13 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

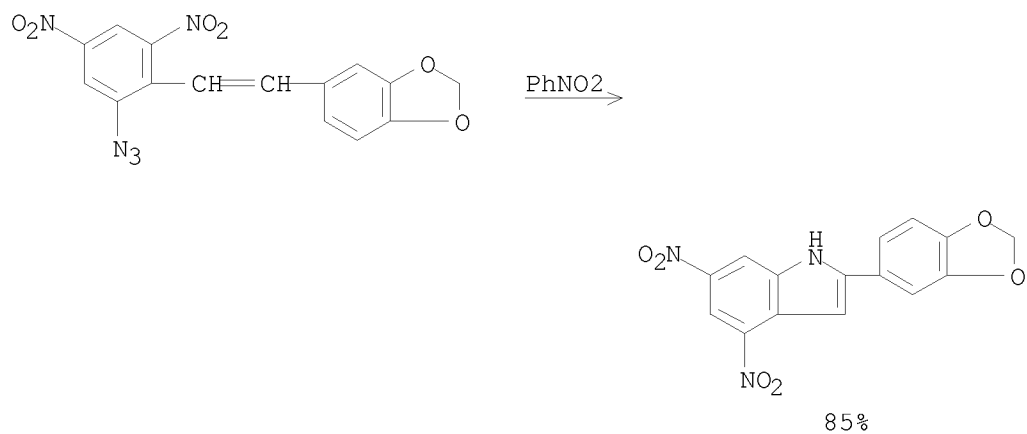
RX(4) OF 5



REF: Journal of Molecular Catalysis A: Chemical, 152(1-2), 47-54; 2000

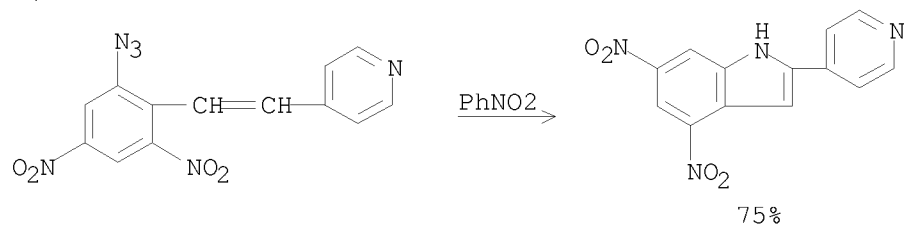
L4 ANSWER 14 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(22) OF 57



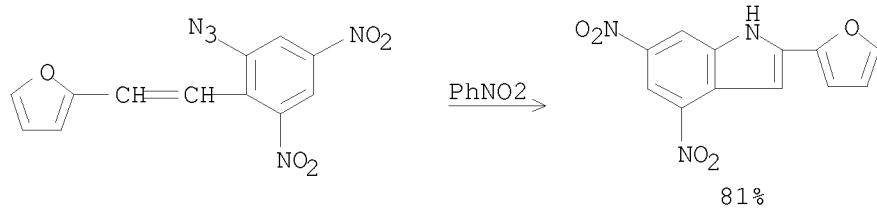
REF: Synthesis, (12), 2065-2070; 1999

RX(24) OF 57



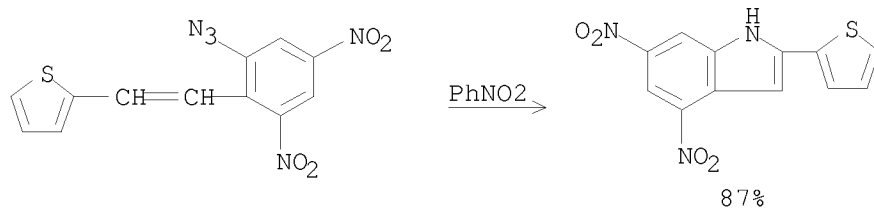
REF: Synthesis, (12), 2065-2070; 1999

RX(25) OF 57



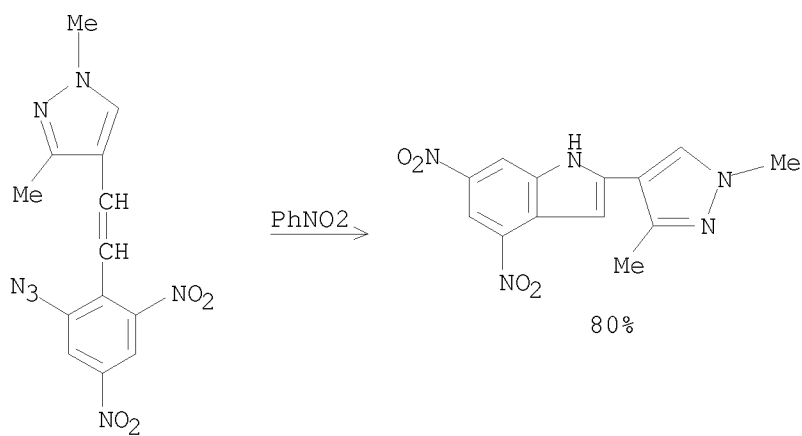
REF: Synthesis, (12), 2065-2070; 1999

RX(26) OF 57



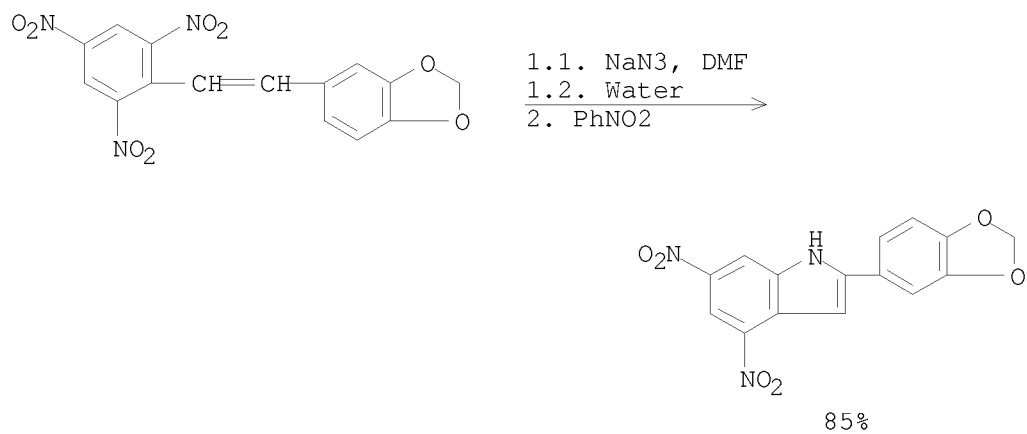
REF: Synthesis, (12), 2065-2070; 1999

RX(28) OF 57



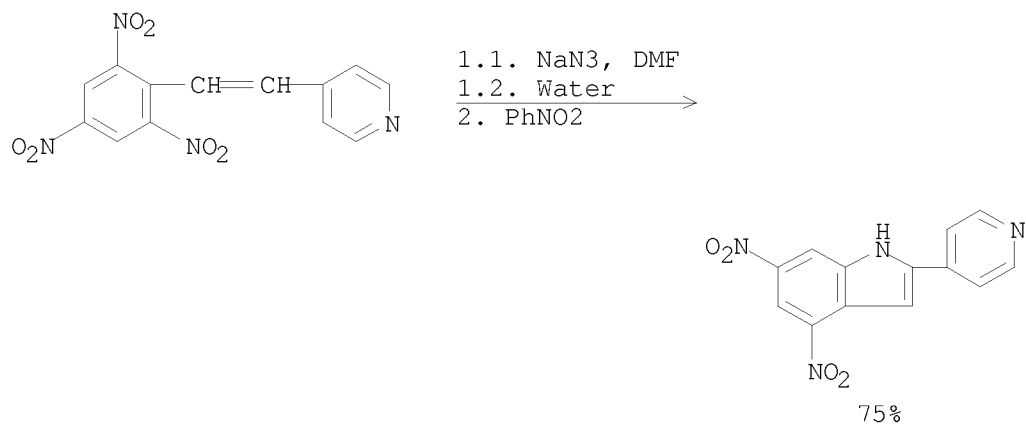
REF: Synthesis, (12), 2065-2070; 1999

RX(41) OF 57 - 2 STEPS



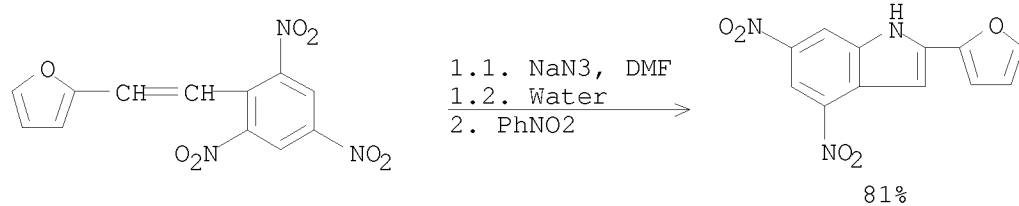
REF: Synthesis, (12), 2065-2070; 1999

RX(43) OF 57 - 2 STEPS



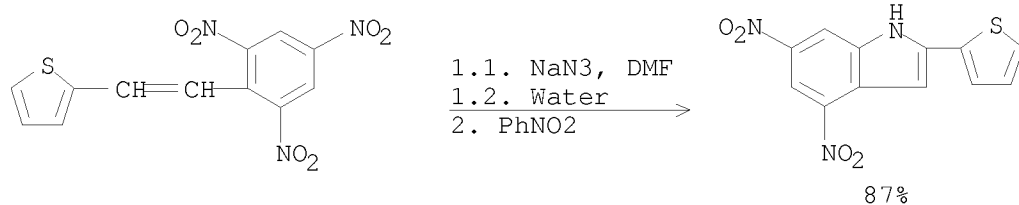
REF: Synthesis, (12), 2065-2070; 1999

RX(44) OF 57 - 2 STEPS



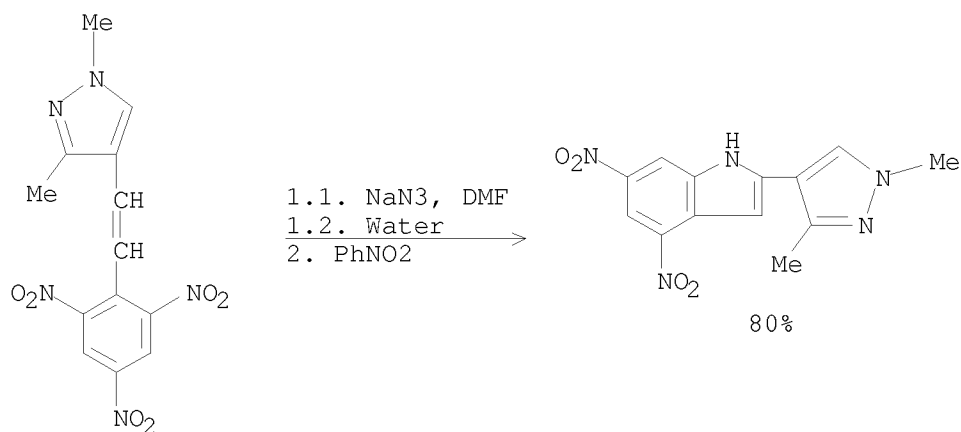
REF: Synthesis, (12), 2065-2070; 1999

RX(45) OF 57 - 2 STEPS



REF: Synthesis, (12), 2065-2070; 1999

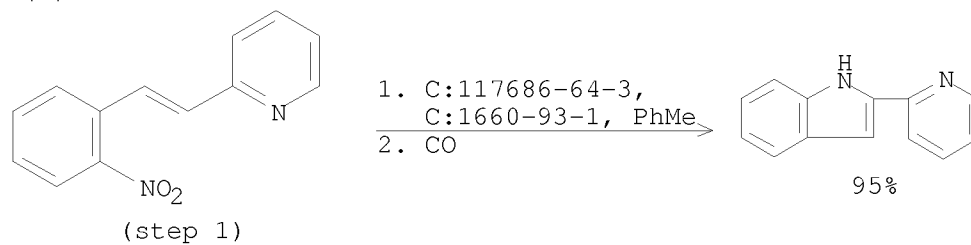
RX(47) OF 57 - 2 STEPS



REF: Synthesis, (12), 2065-2070; 1999

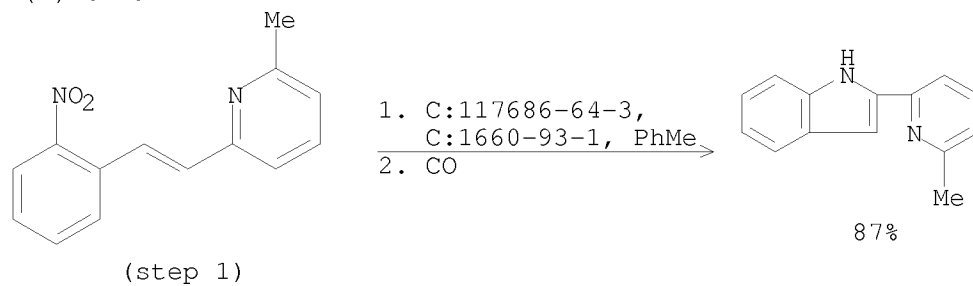
L4 ANSWER 15 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

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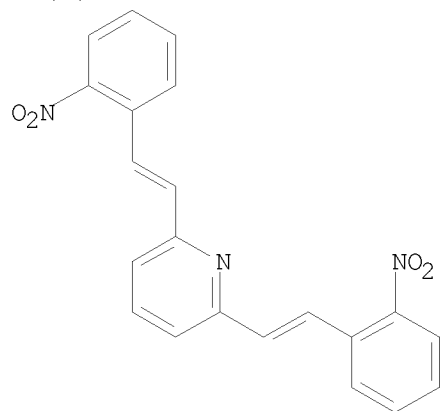
REF: Journal of Molecular Catalysis A: Chemical, 135(3), 241-248; 1998

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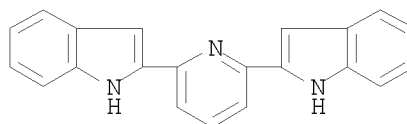
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RX(3) OF 9



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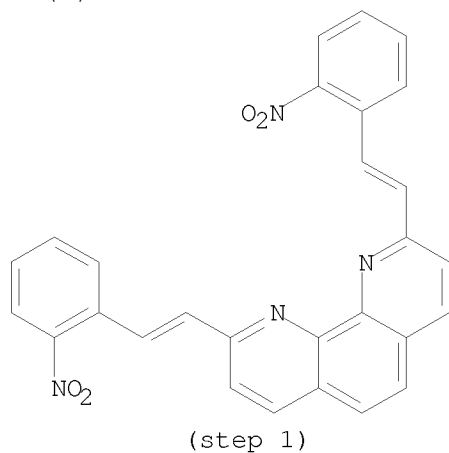
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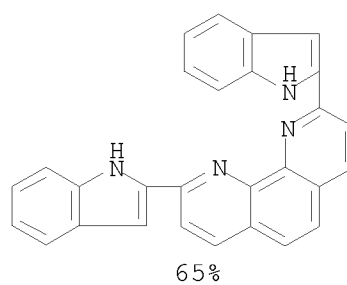
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REF: Journal of Molecular Catalysis A: Chemical, 135(3), 241-248;  
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RX(4) OF 9

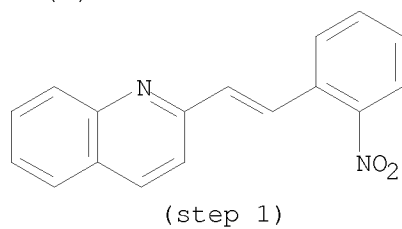


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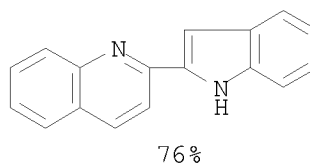


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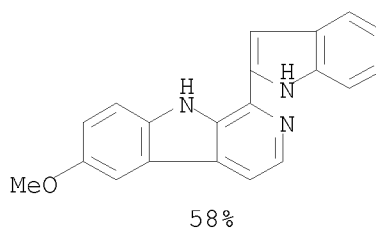
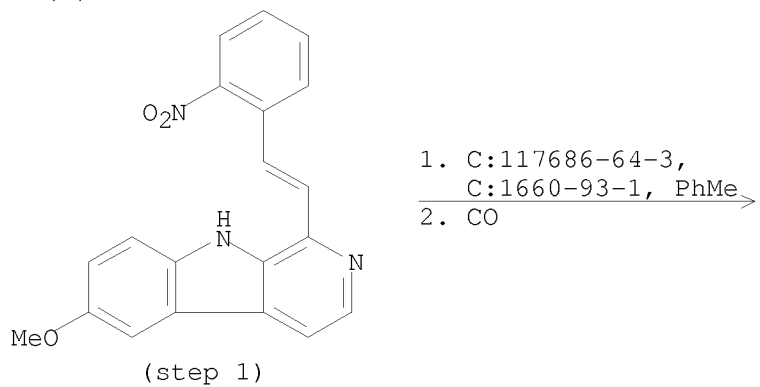


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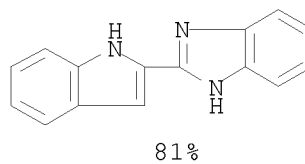
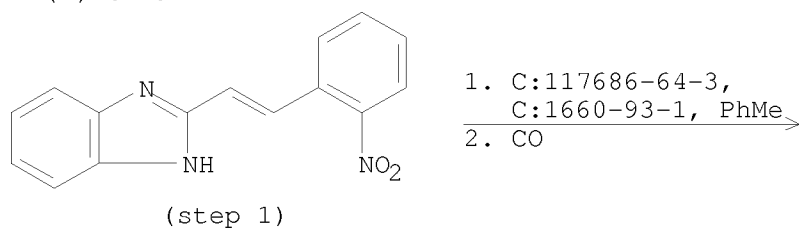
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REF: Journal of Molecular Catalysis A: Chemical, 135(3), 241-248; 1998

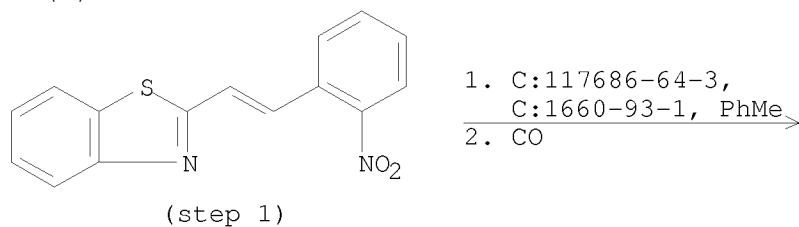
RX(7) OF 9



REF: Journal of Molecular Catalysis A: Chemical, 135(3), 241-248; 1998

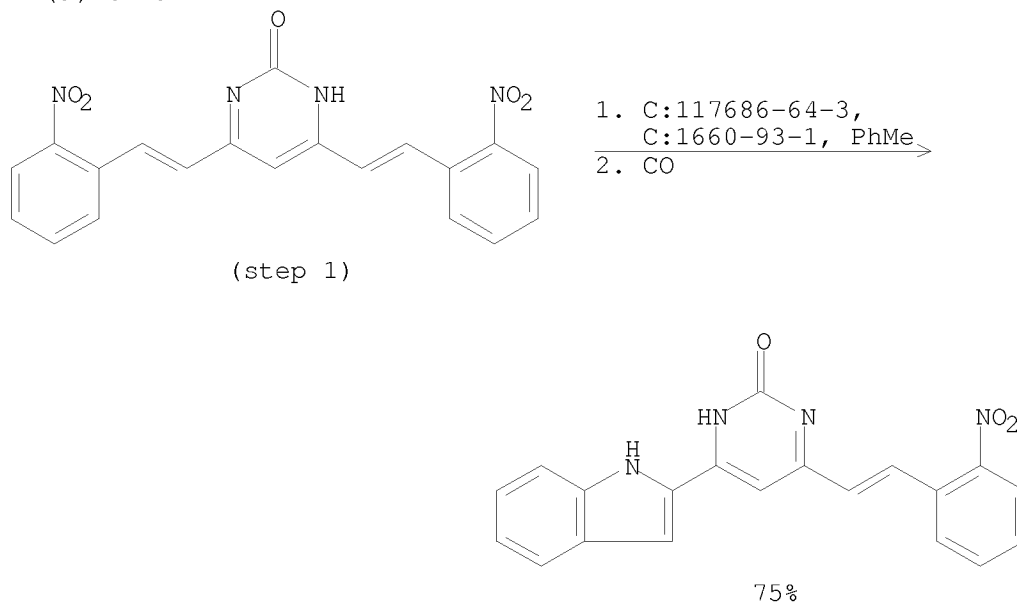


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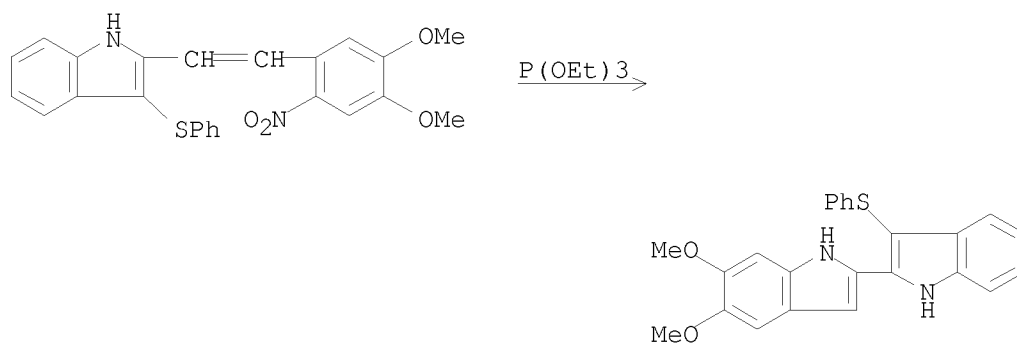
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RX(9) OF 9



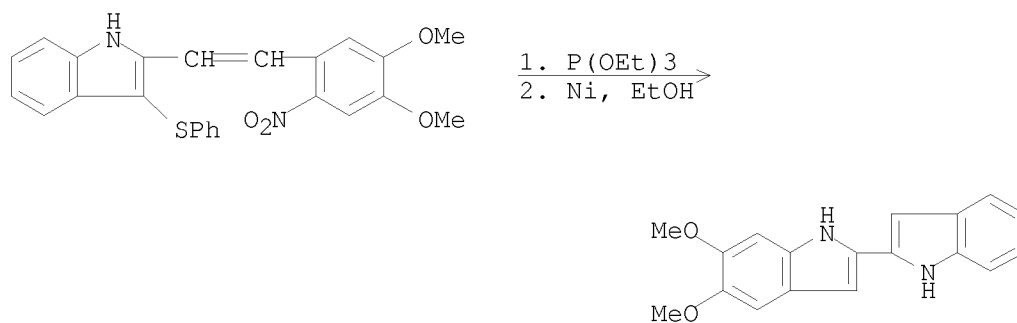
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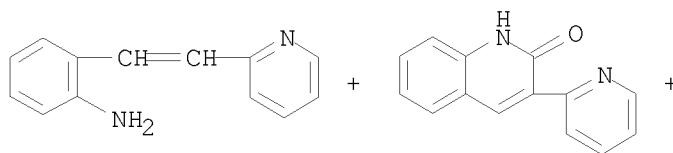
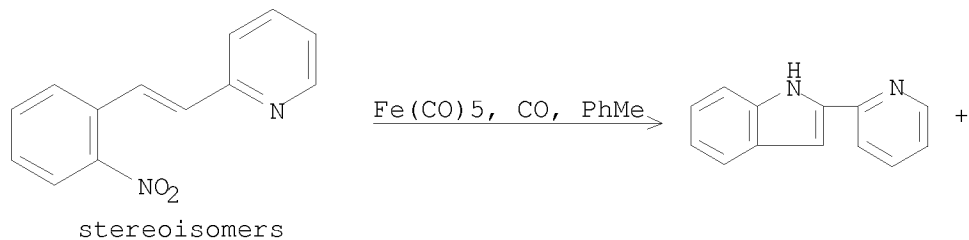
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RX(5) OF 6 - 2 STEPS

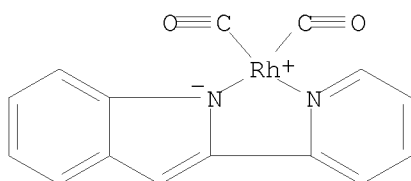


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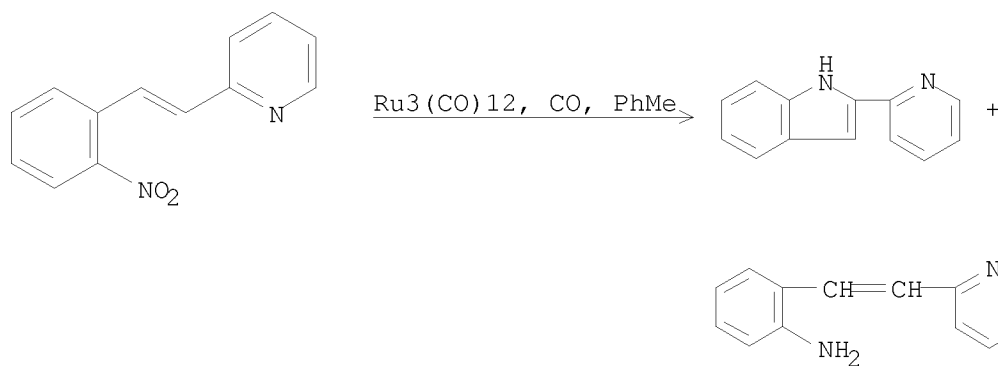


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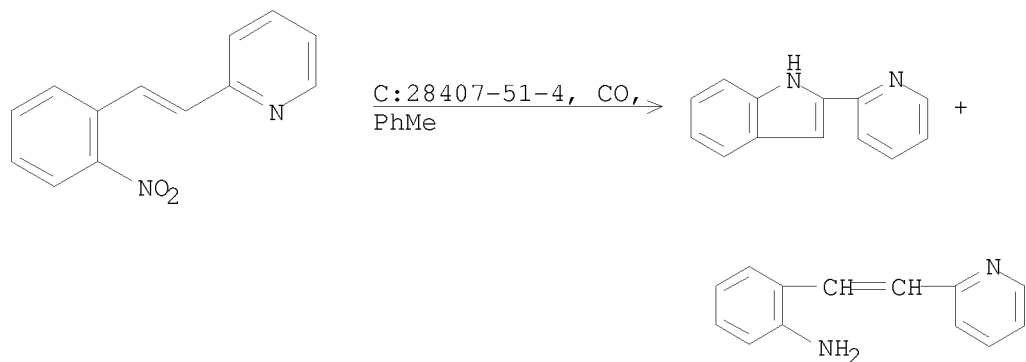
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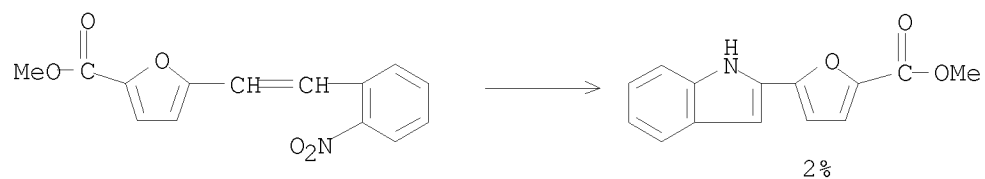
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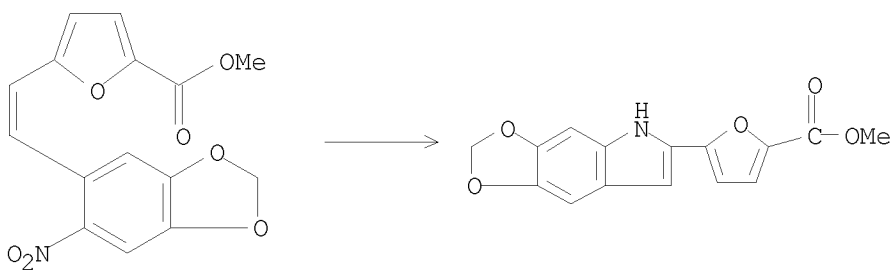
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RX(69) OF 98 - 3 STEPS

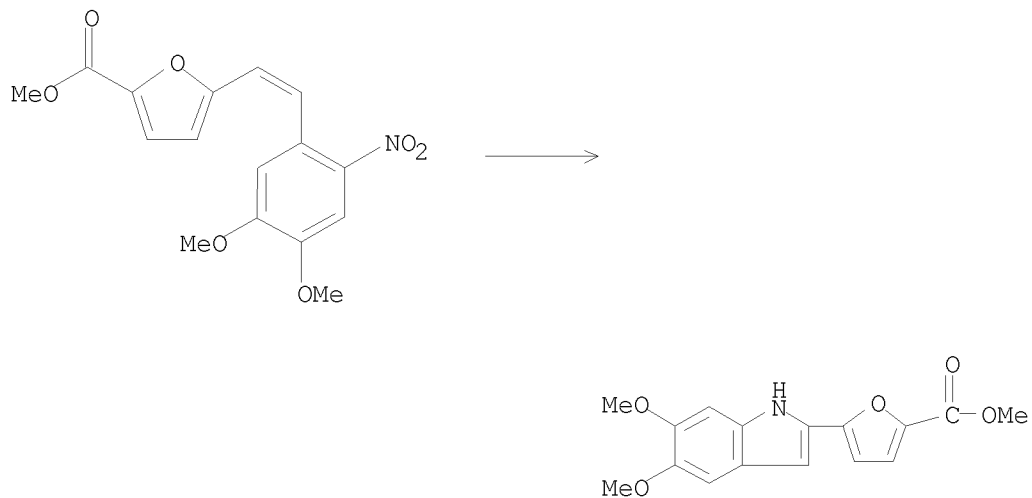


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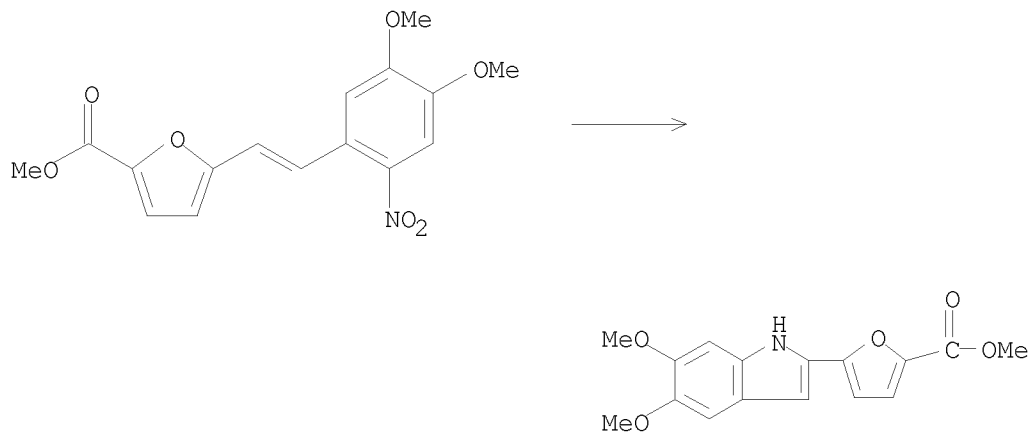
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RX(73) OF 98 - 3 STEPS



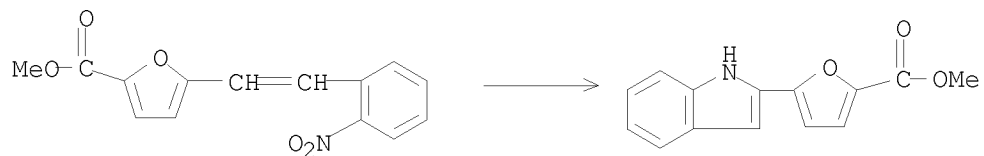
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REF: Chemical & Pharmaceutical Bulletin, 30(1), 140-51; 1982

RX(80) OF 98 - 4 STEPS



REF: Chemical & Pharmaceutical Bulletin, 30(1), 140-51; 1982

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 18:44:53 ON 03 AUG 2008